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(54) Title: THREE-DIMENSIONAL STRUCTURE OF DIPEPTIDYL PEPTIDASE IV

(57) Abstract: A crystal of a dipeptidyl peptidase IV; a three-dimensional structural coordinate of the dipeptidyl peptidase IV; a method for obtaining a three-dimensional coordinate of a homolog protein of the dipeptidyl peptidase IV; a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of the dipeptidyl peptidase IV and a effector of the dipeptidyl peptidase IV; a method for identifying pharmacophore of the effector of the dipeptidyl peptidase IV; a method for designing, identifying, evaluating or searching; the effector, and a program and a medium therefor for use of the three-dimensional structural coordinate.

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DESCRIPTION

THREE-DIMENSIONAL STRUCTURE OF DIPEPTIDYL PEPTIDASE IV

5 TECHNICAL FIELD

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The present invention relates to a crystal and a three-dimensional structural coordinate of a dipeptidyl peptidase IV, and an application thereof. More specifically, the present invention relates to a crystal and a threedimensional structural coordinate, a method for obtaining a three-dimensional structural coordinate of a homolog protein of a dipeptidyl peptidase IV, a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV with an effector (e.g. inhibitor) of the dipeptidyl peptidase IV, a method for identifying a pharmacophore of an effector (e.g. inhibitor) of for the dipeptidyl peptidase IV, a method for identifying sites affecting the activity of the dipeptidyl peptidase IV, a method for designing, identifying, evaluating or searching an effector (e.g. inhibitor) of the dipeptidyl peptidase IV, and a program and a medium therefor for use of the three-dimensional structural coordinate, which are useful in the development of an effector (e.g. inhibitor) of the dipeptidyl peptidase IV, useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like; and an effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like.

BACKGROUND ART

Dipeptidyl peptidase IV (hereinafter also referred to as DPPIV) is a cell membrane protein, which has been found in epithelial cell of small intestine, prostate gland, renal tubule, biliary tract and the like, activated T-cell, B-cell, NK-cell and the like. In the DPPIV, deduced active sites of DPPIV in the C-terminal side are located in extracellular portions and those in the N-terminal side are located in cytoplasm in a living body. Also, there has been suggested the relationship of the above-mentioned DPPIV with the activities of various cytokines such as interleukin-1β, interleukin-2, interleukin-3, interleukin-5, interleukin-6, interleukin-13, tumor necrosis factor-β and the like, and activities of various chemokines such as RANTES and the like in immune system [Rinsho Menneki (Clinical Immunology), 34, Revised and Enlarged Edition 19, 45-53, published by Kagaku Hyoronsha (2000), and the like].

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As to the dipeptidyl peptidase IV, it has been shown that some amino acid residues can be involved in exhibition of the activity of the dipeptidyl peptidase IV by experiments such as biochemical experiments using inhibitors, experiments using mutants produced by site-directed mutagenesis [for example, see Misumi et al, *Biochim. Biophys. Acta*, 1131, 333-336 (1992), Ogata et al, *Biochemistry*, 31, 2582-2587 (1992) and the like].

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However, it is difficult to know the three-dimensional structures for active sites from the information. Therefore, it is presently difficult to obtain the three-dimensional structural information for identifying, searching, evaluating or designing an interaction of the dipeptidyl peptidase IV and a compound that acts with the dipeptidyl peptidase IV on the level of three-dimensional structure and a

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novel compound capable of binding with and acting on the dipeptidyl peptidase IV.

DISCLOSURE OF INVENTION

A first object of the present invention is to provide a crystal of a dipeptidyl peptidase IV, which is useful for providing a three-dimensional structural coordinate as the information for designing, identifying, evaluating or searching an effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. A second object of the present invention is to provide a three-dimensional structural coordinate of the crystal. which can provide the information for designing, identifying, evaluating or searching an effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. A third object of the present invention is to provide a method for obtaining a three-dimensional structural coordinate of a homolog protein of the dipeptidyl peptidase IV, whereby refinement of a three-dimensional structural coordinate of a homolog protein of the dipeptidyl peptidase IV can be more readily performed. Furthermore, a fourth object of the present invention is to provide a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV and an effector (e.g. inhibitor) of the dipeptidyl peptidase IV, which can provide the information for designing, identifying, evaluating or searching an

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effector (e.g. inhibitor) of the dipeptidyl peptidase IV which is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity. biological activity, biological stability, absorbency to a living body, and which can favorably act on the dipeptidyl peptidase IV. A fifth object of the present invention is to provide a method for identifying a pharmacophore of the dipeptidyl peptidase IV and the effector (e.g. inhibitor) of the dipeptidyl peptidase IV, which can provide the information for designing, identifying, evaluating or searching an effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency in a living body, and which can be favorably act on the dipeptidyl peptidase IV. A sixth object of the present invention is to provide a method for designing, identifying, evaluating or searching the effector (e.g. inhibitor) of the dipeptidyl peptidase IV, which can logically and conveniently provide the effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency in a living body (in vivo), and which can be favorably act on the dipeptidyl peptidase IV. A seventh object of the present invention is to provide the effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune

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response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. An eighth object of the present invention is to provide a program and a medium therefor, which can rapidly and conveniently perform design, identification, evaluation or search of the effector (e.g. inhibitor) of the dipeptidyl peptidase IV.

Concretely, the present invention relates to:

- [1] a crystal of a dipeptidyl peptidase IV, having characteristics sufficient to ensure a resolution capable of analyzing its three-dimensional structure up to the side chain level by X-ray crystallographic structural analysis;
- [2] the crystal according to the above [1], wherein the dipeptidyl peptidase IV is a soluble polypeptide comprising a region located at extramembrane in a full-length human dipeptidyl peptidase IV;
- [3] the crystal according to the above [1] or [2], wherein the dipeptidyl peptidase IV is a polypeptide having an amino acid sequence in which a transmembrane region is deleted from the amino acid sequence of SEQ ID NO: 2, and a tag peptide is optionally added to a C-terminal side or N-terminal side thereof;
- [4] the crystal according to any one of the above [1] to [3], wherein the crystal has a space group of $P2_12_12_1$, and a lattice constant of the unit cell of $|a| = 118.0 \pm 5.0$ Å, $|b| = 125.9 \pm 5.0$ Å, $|c| = 136.8 \pm 5.0$ Å, and $\alpha = \beta = \gamma = 90^\circ$, and is orthorhombic;
 - [5] the crystal according to any one of the above [1] to [4], wherein the crystal has the structural coordinate shown in Figure 4;
- 25 [6] the crystal according to any one of the above [1] to [4], wherein the

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crystal has a structural coordinate different from the structural coordinate as shown in Figure 4 via fluctuation of a protein;

- [7] a three-dimensional structural coordinate of a dipeptidyl peptidase IV, comprising the structural coordinate shown in Figure 4;
- 5 [8] a three-dimensional structural coordinate of a dipeptidyl peptidase IV, comprising a structural coordinate different from the structural coordinate as shown in Figure 4 via fluctuation of a protein;
 - [9] the three-dimensional structural coordinate according to the above [8], wherein the fluctuation of a protein is a state that is caused by molecular oscillation or temperature, and exhibits an activity for the dipeptidyl peptidase IV in a living body;
 - [10] the three-dimensional structural coordinate according to any one of the above [7] to [9], wherein the dipeptidyl peptidase IV is a soluble polypeptide comprising a region located at extramembrane in a full-length human dipeptidyl peptidase IV;
 - [11] the three-dimensional structural coordinate according to any one of the above [7] to [10], wherein the dipeptidyl peptidase IV is a polypeptide having an amino acid sequence in which a transmembrane region is deleted from the amino acid sequence of SEQ ID NO: 2, and a tag peptide is optionally added of to a C-terminal side or N-terminal side thereof;
 - [12] a three-dimensional structural coordinate of a region in a dipeptidyl peptidase IV, comprising the three-dimensional structural coordinate of the region selected from the group consisting of the following (a) to (d):
 - (a) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and

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all or a part of a group of the amino acid residues located in the adjacent area of each of the Ser 630, Asp 708 and His 740 in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate;

- 5 (b) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of the amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of amino acids in the group of the amino acid residues located in the adjacent area of each of Ser 630, Asp 708 and His 740, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate,
 - (c) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of the amino acid residues located in the adjacent area of said group of the amino acid residues in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate; and
 - (d) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of amino acid residues comprising amino acids

capable of maintaining physicochemical characteristics physiologically equivalent to each of the amino acids in the group of the amino acid residues located in the adjacent area of said group of the amino acids, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate,

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wherein the region in the dipeptidyl peptidase IV is a region involved in binding or interaction between the dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV;

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[13] the three-dimensional coordinate according to the above [12], wherein the physicochemical characteristic is selected from the group consisting of features in shape of a three-dimensional structure, hydrophobicity, electric charge and pK;

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[14] a method for obtaining a three-dimensional coordinate of a homolog protein of a dipeptidyl peptidase IV, characterized in refining an electron density map of the homolog protein of the dipeptidyl peptidase IV comprising the amino acid sequence of SEQ ID NO: 2, based on all and/or a part of the three-dimensional coordinate of any one of the above [7] to [13], to give a three-dimensional structural coordinate;

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[15] a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV characterized in using all and/or a part of the three-dimensional structural coordinate of any one of the above [7] to [13], to give a three-dimensional structural coordinate;

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[16] a method for identifying pharmacophore of an effector of the dipeptidyl peptidase IV, characterized in identifying the pharmacophore based on all and/or

- a part of the three-dimensional structural coordinate of any one of the above [7] to [13], and the steric conformation of the effector of the dipeptidyl peptidase IV; [17] a method for designing, identifying, evaluating or searching an effector of a dipeptidyl peptidase IV, characterized in designing, identifying, evaluating or searching a compound capable of acting on the dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate of any one of the above [7] to [13];
- [18] the method according to the above [17], wherein the method for designing, identifying, evaluating or searching an effector comprises the steps of:
- (i) identifying a region to be targeted for binding or interaction with the effector in a dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate according to any one of the above [7] to [13] and the steric conformation of the effector of the dipeptidyl peptidase IV;
- 15 (ii) identifying atoms or atomic groups capable of generating in the above region at least one intermolecular interaction selected from the group consisting of covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction and hydrophobic interaction, with the atoms or atomic groups existing in a candidate compound; and
 - (iii) designing a compound based on the information of the above step (i) and/or (ii);
 - [19] the method according to the above [18], wherein the method further comprises the steps of:
- 25 detecting an interaction between the dipeptidyl peptidase IV and the

designed, identified, evaluated or searched candidate compound, wherein when an interaction is detected, the candidate compound is identified as a compound capable of binding to the dipeptidyl peptidase IV, based on a degree of the interaction as an index;

5 [20] the method according to the above [18] or [19], wherein the method further comprises the steps of:

contacting the dipeptidyl peptidase IV with the designed, identified, evaluated or searched candidate compound and measuring the activity of the dipeptidyl peptidase IV,

- wherein when an activity increases or decreases, the designed, identified, evaluated or searched candidate compound is identified as a compound having enhancing action or inhibitory action on the activity of the dipeptidyl peptidase IV, based on a degree of the increase or decrease as an index;
 - [21] an effector of the dipeptidyl peptidase IV obtainable by the method of any one of the above [17] to [20];
 - [22] a program and a medium therefor for use of the three-dimensional structural coordinate of any one of the above [7] to [13], wherein all and/or a part of the three-dimensional structural coordinate of any one of the above [7] to [13] is recorded;
- 20 [23] the program and the medium according to the above [22], comprising a means for identifying, searching, evaluating or designing a compound capable of binding to the dipeptidyl peptidase IV or a compound having an enhancing action or inhibitory action on the activity for the dipeptidyl peptidase IV; and [24] the program and the medium according to the above [23], further comprising a means for displaying a three-dimensional graphic display of a

molecule.

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BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 is a photomicrograph of a crystal of a dipeptidyl peptidase IV, wherein the field of view is 4000 $\mu m \times 3000 \ \mu m$.

Figure 2 is a photograph for X-ray diffraction pattern of a crystal of dipeptidyl peptidase IV.

Figure 3 is a photograph showing a three-dimensional structure of a crystal of a dipeptidyl peptidase IV displayed by the program QUANTA (Accelrys, Inc.).

Figure 4 is a drawing showing a three-dimensional coordinate of a crystal of a dipeptidyl peptidase IV.

BEST MODE FOR CARRYING OUT THE INVENTION

In the present specification, amino acid residues are expressed by using the following abbreviations, which have been adopted by the IUPAC-IUB Commission on Biochemical Nomenclature (CBN). Also, unless explicitly otherwise indicated, the amino acid sequences of peptides and proteins are identified from N-terminal to C-terminal, left terminal to right terminal, the N-terminal being identified as a first residue. Ala: alanine residue; Asp: aspartate residue; Glu: glutamate residue; Phe: phenylalanine residue; Gly: glycine residue; His: histidine residue; Ile: isoleucine residue; Lys: lysine residue; Leu: leucine residue; Met: methionine residue; Asn: asparagine residue; Pro: proline residue; Gln: glutamine residue; Arg: arginine residue; Ser: serine residue; Thr: threonine residue; Val: valine residue; Trp: tryptophane residue;

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Tyr: tyrosine residue; Cys: cysteine residue.

The crystal of the present invention is a crystal of a dipeptidyl peptidase IV, having a characteristic sufficient to ensure a resolution capable of analyzing its three-dimensional structure up to the side chain level by X-ray crystallographic structural analysis.

The "characteristic sufficient to ensure a resolution capable of analyzing three-dimensional structure up to the side chain level" is, for example,

- (1) being in a state that a molecule in a unit cell of a crystal has repeats with high regularity, namely, providing diffraction at high resolution;
- 10 (2) having suitable form and size; it is desired that for example, a crystal has at least one side grown to about 0.2 to about 0.5 mm, preferably a cubic crystal having three sides that have similarly grown, or a needle-shaped crystal having a width or thickness of about 0.2 mm or more;
 - (3) having chemical stability, dynamic stability and physical stability; and the like. In a case of the dipeptidyl peptidase IV, which is a polypeptide having a relatively large molecular weight, the term means characteristics sufficient to ensure a resolution of 3Å or less, preferably 2.8Å or less, more preferably 2.6Å or less.

The dipeptidyl peptidase IV used for the preparation of the crystal of the present invention may have a high purity sufficient for forming the crystal. In the present invention, the dipeptidyl peptidase IV used for the preparation of the crystal includes a soluble polypeptide consisting of a region located at extramembrane in a full-length human dipeptidyl peptidase IV, for example, a polypeptide in which a transmembrane region in the N-terminal side [namely the region including the transmembrane sites (the region containing at least the

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amino acid nos: 1-28 of SEQ ID NO: 2, preferably the region of the amino acid nos: 1-32)] is deleted from the amino acid sequence of a full-length human dipeptidyl peptidase IV of SEQ ID NO: 2, and a tag peptide is optionally added to a C-terminal side or N-terminal side of the amino acid sequence. Concrete examples include (I) a polypeptide in which a transmembrane region in the N-terminal side is deleted from the amino acid sequence of a full-length human dipeptidyl peptidase IV of SEQ ID NO: 2; and (II) a polypeptide in which a tag peptide is added to a C-terminal side or N-terminal side of the polypeptide of the above (I). In the polypeptide, since the transmembrane site is deleted therefrom, the polypeptide has excellent characteristics that anchoring to the membrane can be prevented, and the polypeptide is a secretory type and soluble. The tag peptide is not particularly limited. For example, a polyhistidine peptide (an oligopeptide consisting of 4 to 20 of histidine residues) or the like can be preferably used as the tag peptide.

SEQ ID NO: 2 shows the amino acid sequence of a full-length dipeptidyl peptidase IV of human colon.

The full-length dipeptidyl peptidase IV means a polypeptide of a dipeptidyl peptidase IV containing a region comprising a transmembrane site in the N-terminal side. The full-length dipeptidyl peptidase IV includes a polypeptide comprising the amino acid sequence of SEQ ID NO: 2, without being limited thereto, and encompasses its naturally occurring variant, artificially modified variant, a homolog and an ortholog derived from heterogeneous organism, and the like.

Concretely, the full-length dipeptidyl peptidase IV, besides the polypeptide comprising the amino acid sequence of SEQ ID NO: 2, includes

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conservative substitution variants, naturally occurring allelic variants and the like. Also, the full-length dipeptidyl peptidase IV includes a polypeptide having at least one, namely one or more conservative amino acid substitutions, as compared to the polypeptide comprising the amino acid sequence of SEQ ID NO: 2.

The polypeptide as described above may be a polypeptide having biological activities (namely dipeptidyl peptidase IV activity) similar to the polypeptide comprising the amino acid sequence of SEQ ID NO: 2. Concretely, there are included, for instance, a polypeptide having homology of usually about 80% or more, preferably about 90% or more, more preferably about 95% or more on the amino acid level, as compared to the full-length amino acid sequence of SEQ ID NO: 2; a polypeptide encoded by a nucleic acid capable of hybridizing with a nucleic acid consisting of the nucleotide sequence of SEQ ID NO: 1 (nucleotide sequence encoding a full-length dipeptidyl peptidase IV of human colon), under stringent conditions, or a complement thereof; and a polypeptide having deletion, substitution or addition of at least one amino acid, namely one or plural amino acids, preferably one or several amino acids in the amino acid sequence of SEQ ID NO: 2.

The number of deletion, substitution or addition of the amino acids may be to an extent that the biological activities [namely, dipeptidyl peptidase IV activity] are not lost, usually in the number of 1 to about 150, preferably 1 to about 75, more preferably 1 to about 40.

The crystallization is carried out by making a solution containing the desired protein (referred to as a protein solution) supersaturated state, based on the characteristics that the protein in solution state converts to non-soluble state

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and precipitates as a crystal when specific conditions are satisfied. Concretely, the protein can be precipitated by the following procedures 1. or 2.:

- 1. elevating the effective concentration of the protein:
- concretely, adding a precipitant such as a salt, polyethylene glycol or an organic solvent to a protein solution; reducing an amount of a solvent in the protein solution by evaporation or the like; or the like.
- 2. reducing a repulsive force, or increasing an attractive force between protein molecules:

concretely, adding an organic solvent such as an alcohol to a protein solution; changing a hydrogen ion concentration (pH) or temperature of the protein solution; or the like.

As the conditions for the crystallization, physical and chemical factors such as a hydrogen ion concentration (pH), a kind of buffer used and a concentration thereof, a kind of a precipitant added and a concentration thereof, protein concentration, salt concentration, temperature and the like can be involved. A method for controlling and investigating the factors includes batch methods, dialysis methods, vapor diffusion methods (hanging-drop method, sitting-drop method and the like) and the like, described, for instance, in Blundell, T. L. et al., *PROTEIN CRYSTALLOGRAPHY*, 59-82 (1976), published by Academic Press, or the like.

The method for crystallization includes the batch methods, dialysis methods, vapor diffusion methods and the like. By the above method, physical and chemical factors such as a hydrogen ion concentration (pH), a kind and a concentration of the buffer used, and a kind and a concentration of the precipitant used, and physical and chemical factors such as protein concentration, salt

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concentration and temperature can be also determined.

The hydrogen ion concentration (pH) can be adjusted with a buffer. It is desired that the buffer is a buffer having buffering action in a broad range of pH, and being capable of suppressing precipitation of a non-proteinous crystal between the co-existing ion in the solution used during crystallization and the precipitant or the like. The buffer includes Tris-hydrochloric acid buffer, phosphate buffer, cacodylate buffer, acetate buffer, citrate buffer, glycine buffer and the like.

The precipitant may be a substance capable of elevating an effective concentration of the protein or changing a hydrogen ion concentration (pH) of the protein solution. Generally, the precipitant includes salts such as ammonium sulfate, sodium sulfate, sodium phosphate, potassium phosphate, sodium citrate, ammonium citrate, sodium chloride, potassium chloride and ammonium chloride; polyethylene glycols having various average molecular weights of about 200, about 1000, about 2000, about 4000, about 6000, about 8000, about 20000 or the like; organic solvents such as 2-methyl-2,4-pentadiol, methanol, ethanol, isopropanol, butanol and acetone, and the like.

The protein concentration may be a concentration suitable for crystallization, and it is desired that the protein concentration is, for example, 1 to 50 mg/ml, preferably 5 to 20 mg/ml, more preferably 7 to 15 mg/ml.

It is desired that the temperature conditions are 3° to 25°C, preferably 12° to 22°C.

In the case where the crystallization is carried out by the batch method, the crystallization can be carried out by gradually adding a precipitant solution comprising a precipitant, buffer and the like, so as to form a layer on the top layer of the solution containing the dipeptidyl peptidase IV to give a mixture, or by gradually adding the solution comprising the dipeptidyl peptidase IV, so that the solution is an upper layer of the precipitant solution to give a mixture. Here, the mixture is allowed to stand in a tightly closed vessel.

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In the case where the crystallization is carried out by the dialysis method, the crystallization can be carried out by placing a solution comprising dipeptidyl peptidase IV in a size exclusion semi-permeable membrane, and placing a precipitant solution outside of the size exclusion semi-permeable membrane as a reservoir solution, thereby diffusing the reservoir solution to the solution comprising the dipeptidyl peptidase IV via the semi-permeable membrane.

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In the case where the crystallization is carried out by the hanging-drop method in the vapor diffusion method, the crystallization can be carried out by placing a mixed solution of a solution comprising the dipeptidyl peptidase IV and a precipitant solution in a closed vessel allowing to be hanged at a position above the upper space of a reservoir in which the precipitant solution is contained as a reservoir solution, wherein the vapor pressure of the reservoir solution in the reservoir is set to be lower than that of the mixed solution.

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In the case where the crystallization is carried out by the sitting-drop method in the vapor diffusion method, the crystallization can be carried out by placing a mixed solution comprising a solution comprising the dipeptidyl peptidase IV and a precipitant solution in a closed vessel at a position higher than the liquid surface of a reservoir in which the precipitant solution is contained as a reservoir solution, wherein the vapor pressure of the reservoir solution in the reservoir is set to be lower than that of the mixed solution.

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The crystallization can be carried out by the sitting-drop method from the

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viewpoint of obtaining excellent-quality and large crystal.

When the obtained crystal is a crystal insufficient to ensure the X-ray structural analysis, the crystal may be grown by a seeding method such as macroseeding method or micro-seeding method, using the obtained crystal as a seed crystal.

When the macro-seeding method is performed, it is desired that the seed crystal is a single crystal that can be isolated by procedures under microscope wherein the seed crystal has excellent external form (having excellent crystallinity). Also, it is desired that the seed crystal is washed with a drop of a solution obtained by diluting the precipitant, for example, by 0.5 to 1.0-fold. It is desired that the solution used for seeding of the seed crystal is a protein solution having a degree of supersaturation that the crystal grows but the crystal nuclei do not grow. On the other hand, when the micro-seeding method is performed, the form and size of the seed crystal are not particularly limited.

The sequence information for the dipeptidyl peptidase IV and cDNA encoding the dipeptidyl peptidase IV can be obtained from a known information source [GenBank/EMBL accession No: X60708; Misumi et al., *Biochim. Biophys. Acta*, 1131, 333-336, (1992); GenBank/EMBL accession No: M80536; Darmoul et al., *J. Biol. Chem.*, 267, 4824-4833, (1992)]. Therefore, the dipeptidyl peptidase IV or a soluble polypeptide thereof can be produced by using conventional means for gene engineering on the basis of the above sequence information.

The nucleic acid used for production of the dipeptidyl peptidase IV or a soluble polypeptide thereof may be any nucleic acid in which the encoded polypeptide exhibits a dipeptidyl peptidase IV activity. For example, a nucleic

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acid encoding a polypeptide consisting of the amino acid sequence in which a transmembrane region in the N-terminal side (a region containing at least the amino acid nos: 1-28, preferably the region of the amino acid nos: 1-32) is deleted from the full-length human dipeptidyl peptidase IV, and a tag peptide is optionally added to a C-terminal side or N-terminal side of the amino acid sequence.

The nucleic acid can be obtained by, for instance, obtaining a fragment comprising a nucleic acid encoding a full-length dipeptidyl peptidase IV or a part thereof by means of conventional DNA recombination technique, and appropriately arranging the obtained fragment.

SEQ ID NO: 1 shows a sequence of a nucleic acid encoding a full-length dipeptidyl peptidase IV of human colon.

The nucleic acid (DNA or RNA) encoding a full-length dipeptidyl peptidase IV includes, for instance, a nucleic acid comprising human nucleic acids comprising the nucleotide sequence of SEQ ID NO: 1 without being limited thereto, and includes its naturally occurring variant, artificially modified variant, a homolog or ortholog derived from heterogeneous organism.

In other words, besides the nucleic acid comprising the nucleotide sequence of SEQ ID NO: 1, the nucleic acid includes a nucleic acid capable of hybridizing with a nucleic acid comprising the nucleotide sequence of SEQ ID NO: 1 under stringent conditions, more preferably under high-stringent conditions), or a complement thereof (nucleic acid having a complementary sequence).

Concrete examples of the nucleic acid described above include, for instance, a nucleic acid having usually about 70% or more, preferably about 80%

or more, more preferably about 85% or more, still more preferably about 90% or more, still more preferably about 95% or more, homology to the nucleotide sequence of SEQ ID NO: 1, and it is preferable that the polypeptide encoded by the above nucleic acid has a dipeptidyl peptidase IV activity.

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The dipeptidyl peptidase IV activity can be measured by, for example, incubating in a 1.5 ml reaction mixture [composition: 1.5 mM substrate (Gly-Pro-paranitroanilide), 71 mM glycine-NaOH (pH 8.7)] at 37°C for 10 minutes, and determining the liberated paranitroanilide at the absorbance of 405 nm. One unit (1 U) of a dipeptidyl peptidase IV is defined as an amount of the enzyme required for liberating 1 µmol of paranitroanilide per 1 minute.

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In the present invention, the hybridization under stringent conditions can be carried out as normal stringent conditions by performing hybridization in a hybridization solution having a salt concentration of $6 \times SSC$ or an equivalent concentration thereto, under the temperature conditions of 50° to $70^{\circ}C$ for about 16 hours, and optionally performing pre-washing with a solution having a salt concentration of $6 \times SSC$ or an equivalent concentration thereto, and thereafter performing washing with a solution having a salt concentration of $1 \times SSC$ or an equivalent concentration thereof. Furthermore, as the conditions having still higher stringency (high-stringent conditions), the hybridization can be carried out by washing with a solution having a salt concentration of $0.1 \times SSC$ or an equivalent concentration thereto in the above method.

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The dipeptidyl peptidase IV used for the crystallization has purity that can form a crystal, and the purity can be confirmed by conventional means of confirming purity (for example, a method comprising electrophoresing a fraction by polyacrylamide gel electrophoresis, SDS-polyacrylamide gel electrophoresis

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or the like, and visualizing the fraction by silver staining, or the like).

The X-ray structural analysis data of the crystal can be obtained by subjecting the crystal of the present invention to an X-ray crystallographic structural analysis known to one of ordinary skill in the art [for example, see Blundell, T. L. et al., PROTEIN CRYSTALLOGRAPHY, 59-82 (1976), published by Academic Press, and the like, whereby a three-dimensional structural coordinate (a value showing the relationship of the spatial positions of each atom) and a three-dimensional structure model for the crystal can be obtained. Concretely, the three-dimensional structural coordinate of the dipeptidyl peptidase IV is obtained as an atomic coordinate by procedures comprising the steps of 1) irradiating the crystal of the present invention with a monochromatic X-ray to give an X-ray diffraction pattern, 2) obtaining X-ray diffraction intensity data from the X-ray diffraction pattern, 3) obtaining an electron density map by Fourier transform, and 4) allocating a polypeptide chain and side chain thereof on the electron density map based on the amino acid sequence of the polypeptide used for the crystal. Furthermore, the three-dimensional structure is clarified by molecule-modeling based on the three-dimensional structural coordinate. Therefore, the three-dimensional structural coordinate of the dipeptidyl peptidase IV obtained from the crystal of the present invention is also encompassed within the scope of the present invention.

The crystallographic parameters for the crystal are obtained from the X-ray diffraction intensity data of the crystal of the present invention. The crystal of the present invention is an orthorhombic crystal having a space group of $P2_12_12_1$, and a lattice constant of the unit cell of $|a| = 118.0 \pm 5.0$ Å, $|b| = 125.9 \pm 5.0$ Å, $|c| = 136.8 \pm 5.0$ Å, and $\alpha = \beta = \gamma = 90^{\circ}$. The crystal has a

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2.6Å resolution by X-ray crystallographic structural analysis, that is, the crystal has characteristics sufficient to ensure a resolution capable of analyzing up to the side chain level of the polypeptide.

It is a known fact to one of ordinary skill in the art that the same protein can be crystallized even under different conditions. Therefore, the present invention is not limited to only the conditions for crystallization, and the crystal that shows substantially the same crystallographic constants as those in the present invention are also encompassed within the scope of the present invention.

More concretely, the crystal of the dipeptidyl peptidase IV of the present invention has a structural coordinate as shown in Figure 4, or a structural coordinate different from the structural coordinate as shown in Figure 4 via fluctuation of a protein.

The crystal according to the present invention can also be used as a seed crystal for carrying out the crystallization of a polypeptide having a three-dimensional structure similar to that of the dipeptidyl peptidase IV used for, for example, carrying out the crystallization of the dipeptidyl peptidase IV, dipeptidyl peptidase IV-like proteins, homolog proteins and the like, which are derived from other organism species.

When the crystal of the present invention is irradiated with X-ray, a low-temperature measurement may be carried out, as described in Examples set forth below.

The X-ray structural analysis data are converted to a structure factor by evaluating the intensity of X-ray diffraction using MOSFILM Program Package (Version 6.1). Also, in order to obtain the information for the phase, multiple isomorphous replacement method or the like can be performed, for example, as

described in Examples.

In the structural analysis, CCP4 (Collaborative Computational Project, Number 4, 1994, "The CCP4 Suite: Programs for Protein Crystallography," Acta Cryst. D50, 760-763) program or the like is used.

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The three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention can be obtained, for example, as follows. Firstly, Fourier transform calculation is carried out using the differences between the diffraction intensity obtained from two kinds of isomorphous replacement crystals of mercury and the diffraction intensity obtained from native crystal, and investigating the large peaks provided by the heavy atoms (mercury) on the Patterson's diagram to determine the locations of each mercury atoms in the unit cell of the real space. The phase of the crystal structure factor for the native crystal is determined using the obtained location coordinate for the mercury atoms. Furthermore, refinement is performed using the crystal structure factor of the native crystal and two kinds of the crystal structure factors of the isomorphous replacement crystals of mercury, and the coordinate for each of the mercury atoms is more accurately determined. An electron density map for the crystal of the dipeptidyl peptidase IV in the real space is obtained using the phase of the crystal structure factor of the native crystal calculated from the refined mercury atoms coordinate. Furthermore, the electron density map is improved by performing smoothing and histogram matching for the electron density map of the solvent region, whereby an electron density map necessary and sufficient for building a molecular model can be obtained. Next, the sites corresponding to the amino acid residues of the dipeptidyl peptidase IV on the electron density map are identified using QUANTA (manufactured by Accelrys, Inc.) to build the

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molecular model to give a three-dimensional structural coordinate.

The three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention is shown in Figure 4. Figure 4 shows the obtained three-dimensional structural coordinates, according to the format of the Protein Data Bank, which is a notation generally used by one of ordinary skill in the art.

The three-dimensional structural coordinates shown in Figure 4 are those represented using the origin of the unit cell of the crystal as the origin of the three-dimensional space. The R factor that is considered as an index for the accuracy of the obtained molecular model is 24.89%, and the free R factor is 30.15%. In addition, the deviation in the interatomic bond distance from the ideal state of the three-dimensional structure (rms-deviation) and the deviation in the bond angle are 0.006Å and 1.305°, respectively. In the case, for instance, the three-dimensional structural coordinate of the present invention is used for the calculation by a computer, a novel structural coordinate obtained as a result of the operation for mathematical transfer, such as translation, rotation, or symmetry in the three-dimensional space without changing the relative configuration of the atoms, is also encompassed within the scope of the present invention. Furthermore, not only all of the three-dimensional structural coordinate of the present invention but also a part thereof are also encompassed within the scope of the present invention.

The three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention can be used, for example, as shown in Figure 3, for three-dimensional graphic displaying of the stereogram of the three-dimensional structure model, and for evaluation of the structure-activity relationship and the quantitative structure-activity relationship. Also, the structural features of the

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crystal of the present invention can be more concretely shown using the threedimensional structural coordinate shown in Figure 4. The evaluation of the structure-activity relationship or quantitative structure-activity relationship by the three-dimensional structure model is also encompassed within the scope of the present invention.

According to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, one of the characteristics of the dipeptidyl peptidase IV can be found in that the dipeptidyl peptidase IV has 273 molecules of bond water in an asymmetric unit and has 5 molecules of N-acetylglucosamine residues per 1 molecule of the dipeptidyl peptidase IV.

According to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information for atoms or atomic groups of the side chain of the dipeptidyl peptidase IV, interacting with the atoms or atomic groups of a known effector of the dipeptidyl peptidase IV via an intermolecular interaction can be obtained.

Furthermore, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information of regions in the dipeptidyl peptidase IV that are susceptible to binding or intermolecular interaction with the effector can be obtained.

In addition, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information of the structure specific to the dipeptidyl peptidase IV, which is not found in proteins other than the dipeptidyl peptidase IV, can be obtained. Therefore, higher selectivity in the effector targeting a protein other than the dipeptidyl peptidase IV can be designed, when the effector also acts on the dipeptidyl peptidase IV.

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The intermolecular interaction includes covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction, hydrophobic interaction and the like.

In the present specification, the atoms or atomic groups of the effector and atoms or atomic groups of the side chain of the dipeptidyl peptidase IV, which interact with each other via intermolecular interaction, are referred to as "pharmacophore."

Also, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information for the structure specific for the dipeptidyl peptidase IV, which is not found in proteins other than the dipeptidyl peptidase IV, can be provided.

In addition, for example, when the measurement conditions are different in X-ray diffraction, or the three-dimensional structure of the complex in the solution is analyzed using multidimensional NMR, and the like, the three-dimensional structural coordinate may differ from that shown in Figure 4. The three-dimensional structural coordinate varies depending on the fluctuation of protein and the like, and is encompassed within the scope of the present invention.

In the present specification, the "fluctuation of protein" means a state that is caused by molecular oscillation, temperature and the like, and accompanied with the structural change that can exhibit an activity for the dipeptidyl peptidase IV in a living body.

Also, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, one of the characteristics of the dipeptidyl peptidase IV resides in that the amino acid residues, Ser 630, Asp 708

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and His 740, which are involved in the activity deduced by experiments by using various active inhibitors of the dipeptidyl peptidase IV, exist in the adjacent area, even though the amino acid residues exist in distant locations on the primary sequence. Concretely, the distance between the $O_{\delta 2}$ atom of Asp 708 and the $N_{\delta 1}$ atom of His 740, and the distance between the N_{E2} atom of His 740 and the O_y atom of Ser 630 are distances that can form hydrogen bonding.

Therefore, the present invention also includes a three-dimensional structural coordinate of the region in the dipeptidyl peptidase IV, which is involved in binding or interaction of the dipeptidyl peptidase IV with an effector thereof, including a three-dimensional structural coordinate of a region selected from the group consisting of the following (a) to (d):

(a) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of amino acid residues located in the adjacent area of each of the Ser 630, Asp 708 and His 740 in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate;

a region characterized by Ser 630, Asp 708 and His 740 in the amino acid

(b) sequence of SEQ ID NO: 2, and all or a part of a group of amino acid residues comprising amino acids 20 capable of maintaining physicochemical characteristics physiologically equivalent to each of amino acids of the group of amino acid residues located in the adjacent area of each of Ser 630, Asp 708 and His 740, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate, 25

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- aregion characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of amino acid residues located in the adjacent area of said group of the amino acid residue in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate; and
- (d) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and

all or a part of a group of amino acid residues of a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to the each amino acid of the amino acid residues located in the adjacent area of said groups of the amino acids, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate.

In the present specification, the "adjacent (area)" refers to an area involved in covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction, hydrophobic interaction or the like with the amino acid residues, concretely, a region within 10Å, preferably within 8Å, more preferably within 5Å.

The physicochemical characteristic includes features in shape of the three-dimensional structure, hydrophobicity, electric charge, pK and the like.

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The "amino acid capable of maintaining physicochemical characteristics physiologically equivalent" may be an amino acid analogue residue obtained by replacing a side chain of amino acid residues in the three-dimensional structural coordinate shown in Figure 4 with other side chain, for example, showing bioisosterism. Alternatively, the amino acid residue in the three-dimensional structural coordinate shown in Figure 4, may be replaced with another amino acid residue belonging to the same Group, in any of the following Groups I to VI:

- I glycine, alanine;
- 10 II valine, isoleucine, leucine;
 - III aspartic acid, glutamic acid, asparagine, glutamine;
 - IV serine, threonine;
 - V lysine, arginine;
 - VI phenylalanine, tyrosine.

According to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, a three-dimensional structural coordinate of a polypeptide can be easily derived if an accurate amino acid sequence is determined, even when the polypeptide is a dipeptidyl peptidase IV or a dipeptidyl peptidase IV-like protein derived from other organism species, as long as the polypeptide is a polypeptide having high homology on the level of amino acid sequence with the dipeptidyl peptidase IV used for the preparation of the crystal of the present invention (for example, at least 20%, preferably 30% or more, more preferably 40% or more).

Furthermore, the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention can be used for X-ray crystallographic

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structural analysis of the crystal and the like of other proteins having an amino acid sequence with significant homology with the dipeptidyl peptidase IV used for the preparation of the crystal of the present invention. Concretely, according to the molecular replacement method [for example, see Blundell, T. L. et al., PROTEIN CRYSTALLOGRAPHY, 446-464 (1976), published by Academic Press and the like], the three-dimensional structural coordinate thereof can be quickly and readily obtained from the structure factors obtained by the X-ray diffraction pattern of the crystal, without using multiple isomorphous replacement method, even for the determination of the structural coordinate of the above-mentioned crystal of which structural coordinate has not yet been known.

In the present specification, the term "significant homology" is a case where there is identity of 20%, or more, preferably by 30% or more, between the amino acid sequences.

When the molecular replacement method is performed, for example, a program such as X-PLOR and CNX (both manufactured by Accelrys Inc.) or AMORE [one of the programs of CCP4 (Collaborative Computational Project, Number 4), *Acta Crystallogr.* **D50**, 670-673 (1994)] can be run by a computer on which the program can be executed. Here, whether or not the molecular replacement method is applicable can be determined by actually applying the molecular replacement method to the structure factors calculated from the X-ray diffraction pattern of the desired crystal and obtaining a significant solution.

In other words, the three-dimensional structural coordinate obtained by structural analysis by molecular replacement method is encompassed within the scope of the present invention as long as a significant solution is obtained. The present invention also encompasses a three-dimensional structural coordinate of

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a dipeptidyl peptidase IV, or a dipeptidyl peptidase IV-like protein, namely a homolog protein or the like of other organism species derived by the above method.

Therefore, according to the present invention, a method for obtaining a three-dimensional structural coordinate of a homolog protein of a dipeptidyl peptidase IV comprising the step of performing refinement of an electron density map of the homolog protein of the dipeptidyl peptidase IV comprising the amino acid sequence of SEQ ID NO: 2, based on the three-dimensional structural coordinate of the present invention, to give a three-dimensional structural coordinate is provided. Also, a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV, based on the three-dimensional structural coordinate of the present invention, is likewise provided.

According to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, a method for identifying a region or site for a target for binding or interaction between the dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV is provided, based on the analysis of the binding regions between the dipeptidyl peptidase IV and a known effector of the dipeptidyl peptidase IV such as an inhibitor, or based on the simulation of the interaction between the dipeptidyl peptidase IV and a known effector of the dipeptidyl peptidase IV.

Also, based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV, the pharmacophore of the effector of the dipeptidyl peptidase IV can be identified. A method for identifying the

pharmacophore is also provided. The method is useful for designing an effector having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermodynamic stability, higher absorbency to a living body, and lower toxicity.

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Concretely, for example, the region or site for a target involved in binding or interaction of the dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV, can be identified by:

- 1) obtaining a crystal of a complex of the dipeptidyl peptidase IV and a known effector of the dipeptidyl peptidase IV such as an inhibitor, and obtaining a three-dimensional structural coordinate of the crystal based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV, whereby obtaining the three-dimensional structural coordinate of a binding region of the dipeptidyl peptidase IV and the effector;
- 2) simulating an intermolecular interaction between the dipeptidyl peptidase IV and a known effector of the dipeptidyl peptidase IV based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV;

or the like.

The crystal of the above-mentioned complex can be obtained by, for example, incubating the crystal of the present invention in a solution comprising the effector, forming a complex of the dipeptidyl peptidase IV and the effector, and crystallizing the obtained complex, and the like.

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Also, when the three-dimensional structural coordinate of the crystal of

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the complex is obtained, the steric structure of the effector of the abovementioned complex can be readily obtained by calculating the differential Fourier diagram utilizing a three-dimensional structure model defined by the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, whereby specific interaction forms and interaction sites between the dipeptidyl peptidase IV and the effector can be readily clarified.

When the intermolecular interaction is simulated, for example, the space regions, residues and the like in which covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction, hydrophobic interaction or the like can be simulated, based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV.

Furthermore, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the three-dimensional structural coordinate or the three-dimensional structure model based on the three-dimensional structural coordinate regarded as an active center of the dipeptidyl peptidase IV, sites indirectly acting on the active center and regions or sites involved in binding or interaction with the effector, or the like, is obtained, whereby a compound capable of specifically acting on the dipeptidyl peptidase IV can be designed, identified, evaluated or searched.

For example, in the structural coordinate of Figure 4 and the threedimensional structure model defined by the structural coordinate, a compound capable of modifying the activity of the dipeptidyl peptidase IV can be designed, identified, evaluated or searched, based on the regions characterized by Ser 630,

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Asp 708 and His 740, and all or a part of amino acid residues of the group of the amino acid residues located in the adjacent area of the Ser 630, Asp 708 and His 740.

Therefore, according to the present invention, a method for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV is provided.

One of the significant features of the method of the present invention for designing, identifying, evaluating or searching an effector resides in that the method comprises designing, identifying, evaluating or searching a compound capable of acting on the dipeptidyl peptidase IV, based on the three-dimensional structural coordinate of the present invention.

According to the method of the present invention for designing, identifying, evaluating or searching an effector, since the method is based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information for a structure specific to the dipeptidyl peptidase IV, which is not found in proteins other than the dipeptidyl peptidase IV can be obtained. Therefore, according to the method of the present invention for designing, identifying, evaluating or searching an effector, the method has an excellent effect that the selectivity of the effector of the dipeptidyl peptidase IV can be enhanced.

Also, according to the method of the present invention for designing, identifying, evaluating or searching an effector, since the method is based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, visual studies and/or energy calculation can be made according to the method by using a computer and the like. Therefore, there are

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exhibited some excellent effects that a compound having excellent characteristics such as having higher avidity, higher biological activity, higher biological stability, higher thermodynamic stability, higher absorbency in a living body, and lower toxicity, than those for a known inhibitor can be designed, identified, evaluated or searched, and that logical design can be performed in the three-dimensional space.

In the present specification, the "effector" includes a compound that inhibits or enhances the activity (i.e. inhibitor or activator), which may be natural compounds or synthetic compounds, or may be polymers or low-molecular weight compounds.

A concrete example of the method of the present invention for designing, identifying, evaluating or searching an effector includes a method comprising the steps of:

- (i) identifying a region to be targeted for binding or interaction with the effector in a dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV;
- (ii) identifying corresponding atoms or atomic groups capable of generating in the region at least one intermolecular interaction selected from the group consisting of covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction and hydrophobic interaction, with the atoms or atomic groups existing in a candidate compound; and
- (iii) designing a compound based on the above information of the above step(i) and/or (ii).

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The three-dimensional structural coordinate used for designing, identifying, evaluating or searching a compound capable of binding to the dipeptidyl peptidase IV may be a coordinate fixed in the three-dimensional space, and the intensity of binding with the compound or the like can be calculated by carrying out translation or rotation in the three-dimensional space, and transfer to an extent that the chemical covalent bond would not be cleaved in the amino acid residues of the dipeptidyl peptidase IV.

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In the above step (i), the "region to be targeted in the dipeptidyl peptidase IV" preferably includes an active center of the dipeptidyl peptidase IV, sites indirectly acting on the active center and the like. For example, there is included a region characterized by Ser 630, Asp 708 and His 740 and all or a part of a group of the amino acid residues located in the adjacent area of Ser 630, Asp 708 and His 740, and the like in the structural coordinate of Figure 4 and the three-dimensional structure model defined by the structural coordinate. The atoms or atomic groups that can be matched therewith are identified, based on the three-dimensional structural coordinate of an active center, sites indirectly acting on the active center and the like, whereby the candidate atoms or candidate atomic groups can be obtained.

In the above step (ii), for example, the atoms or atomic groups capable of associating via intermolecular interaction between the atoms or atomic groups in the region, concretely, the corresponding atoms or atomic groups capable of generating covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction, hydrophobic interaction and the like, are searched and extracted, based on the information identified in the above step (i).

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Next, in the above step (iii), the corresponding atoms or atomic groups searched in the above step (i) and/or (ii) are combined to design a compound.

Thereafter, if desired, whether or not the compound designed in the above step (iii) is matched via intermolecular interaction with the side chains and atoms or atomic groups in the dipeptidyl peptidase IV as defined by the three-dimensional structural coordinate of the present invention can be simulated.

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The compound designed, identified, evaluated or searched by the above steps (hereinafter also referred to as a candidate compound in the present specification) can be obtained by generally used chemical synthetic methods, depending on the compound.

In addition, in the method of the present invention for designing, identifying, evaluating or searching an effector, there can be carried out a step of detecting the interaction between the dipeptidyl peptidase IV and the candidate compound. When the interaction is detected, the interaction serves as an index showing that the above candidate compound is a compound capable of binding to the dipeptidyl peptidase IV.

The above interaction can be detected by, for example, plasmon resonance analysis apparatus, mass spectrometer, titration isothermal calorimetry, NMR and the like. For example, in the case of plasmon resonance analysis apparatus, when a sensorgram indicates the formation of a complex, by contacting the dipeptidyl peptidase IV-immobilized matrix with the candidate compound and performing analysis by optical detection (for example, photometer, polarization photometer and the like) and the like, it would be an index showing that the interaction between the candidate compound and the dipeptidyl peptidase IV is generated. For example, in the case of a mass spectrometer, when a spectrum

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indicates the formation of a complex, by contacting the dipeptidyl peptidase IVimmobilized matrix with the candidate compound and performing analysis with a mass spectrometer (matrix-assisted laser desorption/ionization-time of flight mass spectrometry: MALDI-TOF MS, electro spray-ionization mass spectrometer: ESI-MS and the like), it would be an index showing that the interaction between the candidate compound and the dipeptidyl peptidase IV is generated. For example, in the case of titration-thermal calorimetry interaction analysis, when the titration curve indicates the formation of a complex, by contacting a solution of the dipeptidyl peptidase IV with the candidate compound, and measuring the heat coming in and out of a thermal diode and the like, it would be an index showing that the interaction between the candidate compound and dipeptidyl peptidase IV is generated. For example, in the case of NMR, when a spectrum indicates the formation of a complex, by analyzing by NMR a solution prepared mixing the dipeptidyl peptidase IV and a candidate compound, it would be an index showing that the interaction between the candidate compound and the dipeptidyl peptidase IV is generated.

Furthermore, the method of the present invention for designing, identifying, evaluating or searching an effector may further comprise the steps of contacting the dipeptidyl peptidase IV with a candidate compound, and thereafter measuring the activity of the dipeptidyl peptidase IV. When the dipeptidyl peptidase IV activity increases or decreases, it would be an index showing that the candidate compound is a compound having enhancing action or inhibitory action on the activity of the dipeptidyl peptidase IV.

The dipeptidyl peptidase IV activity can be measured by, for example, incubating a 1.5 ml reaction mixture [composition: 1.5 mM substrate

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(Gly-Pro-paranitroanilide), 71 mM glycine-NaOH (pH 8.7)] at 37°C for 10 minutes in the presence of a candidate compound, and measuring the liberated paranitroanilide at the absorbance of 405 nm. During the measurement of the activity, the candidate compound may be evaluated by using a reaction system in which a suitable dilution series of the compound is added thereto.

The method of the present invention for designing, identifying, evaluating or searching the effector can be performed by, for example, sequentially selecting the interaction between the dipeptidyl peptidase IV and the compounds in a database in a computer to which the structures of plural of compounds had been inputted, or the interaction between the dipeptidyl peptidase IV and the designed compound, by visual methods (visual selection method) utilizing the database; and/or sequentially calculating the avidity with a computer, and searching a compound capable of stably interacting with the dipeptidyl peptidase IV from the database (computer-assisted avidity evaluation method) and the like, based on the three-dimensional structural coordinate of the present invention.

In the above visual selection method, the database of the structures of compounds may be a database in which the three-dimensional structural coordinates have been determined and inputted. Alternatively, in the case of a compound having a low molecular weight, the database may be a database in which the information for chemical covalent bond of a compound having a low molecular weight had been inputted, because the conformation can be relatively freely changed, and the three-dimensional structural coordinate of each conformation can be derived by calculation in a relatively short time.

Concretely, in the visual selection method, the expected complex between the dipeptidyl peptidase IV and a candidate compound or a part thereof is firstly

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displayed on a computer screen, based on the three-dimensional structural coordinate of the present invention. Next, the intermolecular interaction binding between a compound in the database and the binding regions of the dipeptidyl peptidase IV is simulated on the computer, taking chemical interaction into consideration. Also, the simulation of the chemical modification of the compound is performed on the computer, and the changes in the interaction caused as a result thereof are observed on the computer screen. During the simulation, the three-dimensional space can be more easily understood by displaying the three-dimensional structure of the protein on the computer screen so that the structure corresponds to Crystal Eye glasses supplied by Silicone Graphics; simultaneously displaying two screens in which each angle is adjusted for displaying the object, according to the visual fields of the right eye and left eye, which is so-called referred to as "stereovision" which is frequently used by one of ordinary skill in the art; or the like. In addition, the three-dimensional structure can be visually studied by methods other than the stereoscopic displaying of the three-dimensional structure.

The candidate compound capable of generating suitable interaction can be obtained by displaying on a computer a group of candidates with appropriate conformation and selecting an appropriate one therefrom; calculating a structure having a low energy state on a computer; or the like. Next, a derivative of a compound capable of generating more preferable binding with the dipeptidyl peptidase IV may be searched among the candidate compound.

More specifically, on the level of the three-dimensional structure, the followings may be taken into consideration:

25 a group likely to be charged negatively, such as carboxyl group, nitro

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group, or a halogen group in the compound interacts with an amino acid residue having a positive charge, such as lysine, arginine or histidine in the dipeptidyl peptidase IV;

- a group likely to be charged positively, such as amino group, imino group or guanidyl group in the compound interacts with an amino acid residue having negative charge, such as glutamic acid or aspartic acid in the dipeptidyl peptidase IV;
- a hydrophobic functional group such as an aliphatic group or an aromatic group in the compound interacts with a hydrophobic amino acid residue such as alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophane or methionine in the dipeptidyl peptidase IV:
- a group involved in hydrogen bonding, such as hydroxyl group or amide group is allowed to form hydrogen bonding with a main chain or side chain portion;
- a group or an atom likely to be charged negatively, such as carboxyl group, nitro group or a halogen group in the compound interacts with a positively charged atom on a main chain or side chain portion;
 - a group or an atom likely to be charged positively, such as amino group, imino group or guanidyl group in the compound interacts with a negative charged atom on a main chain or a side chain portion;
 - 7 the flexibility of the three-dimensional structure of the compound is lowered by, for instance, cyclizing the linear chain portion;

or the like. For example, a derivative may be designed and synthesized so that the atoms having negative charge of the candidate compound are located in the adjacent region of the side chain of an amino acid residue having positive charge

such as lysine, arginine or histidine, in the amino acid residue of the dipeptidyl peptidase IV, and that an atom having positive charge of the candidate compound is located in the adjacent region of the side chain of the amino acid residue having negative charge such as glutamic acid or aspartic acid in the amino acid residue of the dipeptidyl peptidase IV. Also, a group suitable for forming a hydrophobic interaction may be introduced into the portion capable of forming a hydrophobic interaction between the compound and the dipeptidyl peptidase IV, to design and synthesize a derivative. In addition, a group suitable for forming hydrogen bonding may be introduced into the portion capable of forming hydrogen bonding between the compound and the dipeptidyl peptidase IV, to design and synthesize a derivative. In the above-mentioned designing, it is desirable that van der Waals interaction is as high as possible, and that steric hindrance does not occur between each of the atoms. Furthermore, it is desirable that new void portions are not produced by modification of the compound and that in regions already containing void portions, the void portions are filled as much as possible.

As described above, the design, identification, evaluation or searching of a final compound can be thus performed with visually comprehensively considering intermolecular interaction and other factors on a computer screen.

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In the computer-assisted avidity evaluation method, in order to determine the validity for the designing of a new compound, and to obtain a compound that can stably interact from the compounds in the database, a docking software (DOCK, GOLD, FlexX, Glide or the like) is used for evaluation of binding based on the energy by calculating a molecular force field between the compound and the dipeptidyl peptidase IV, evaluation of binding based on chemical

characteristics, evaluation of binding based on the Protein Data Bank (PDB), and the like. Further, in a model system consisting of the compound and the dipeptidyl peptidase IV, or in a model system further comprising solvent molecules and the like, it can be led to a compound that can stably interact by obtaining the index showing avidity, such as free energy of bonding, the ratio obtained from bond state number and non-bond state number, and the like by using molecular kinetic calculation or Monte Carlo calculation. The programs for calculation of molecular force field and molecular kinetic include AMBER, CHARMm, DISCOVER, PRESTO and the like, and the force field used includes AMBER, CHARMm, OPLS, MMCF, CVFF and the like. Furthermore, a program such as Ludi which automatically outputs the candidates for a candidate compound by providing a three-dimensional structural coordinate of the amino acid residues interacting in the dipeptidyl peptidase IV may be used.

The visual selection method and computer-assisted avidity evaluation method can be performed alone or in combination. In the case of performing the methods in combination, the avidity is actually calculated for the compounds that has been expected to be more desirable in visual investigation, and the validity thereof is evaluated. By repeatedly performing the calculation and evaluation, more excellent compounds may be designed, identified, evaluated or searched.

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Next, the designed, identified, evaluated or searched compound is optimized to be a more excellent compound, such as a compound having more excellent characteristics as a medicament, such as being excellent *in vivo* kinetics, having low toxicity and low side-effect; a compound having a still higher biological activity as an effector; a compound having an advantageous structure as a medicament in view of its oral administration; and the like.

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The resulting candidate compound can be obtained using generally used techniques for chemical synthesis depending on the kind of the compound.

The present invention also encompasses an effector of the dipeptidyl peptidase IV, which is obtained by the method of the present invention for designing, identifying, evaluating or searching an effector. When the effector is a compound capable of inhibiting or enhancing the activity of the dipeptidyl peptidase IV, the effector (inhibitor or activator) is expected to be an agent for, for example, a modulatory agent of immune response, a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like.

The three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention can be provided as a computer program, a medium or the like, which displays the three-dimensional structure of the molecule based on the three-dimensional structural coordinate and can be provided via a telecommunication line or the like. Therefore, using a computer or the like, the three-dimensional coordinate of the dipeptidyl peptidase IV can be displayed in detail, allowing to perform the method of the present invention for designing, identifying, evaluating or searching an effector more rapidly, conveniently and logically.

The present invention also encompasses a program or a medium therefor for use of the three-dimensional structural coordinate, in which all and/or a part of the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention is recorded.

The medium may be any of those in which the three-dimensional structural coordinate of the present invention can be derived on a program that

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runs on a computer, and includes, for instance, electric memory media referred to as memory; semi-permanent memory media such as a FD, a hard disk, an optical disk, an opto-magnetic disk and a magnetic tape, and the like. In addition, the program and the medium therefor for use of the three-dimensional structural coordinate of the present invention also encompass those having a form which can be communicated via a telecommunication line such as internet.

Also, the program and the medium therefor for use of the three-dimensional structural coordinate of the present invention may further comprise a means for displaying the three-dimensional graphic display of the molecule. The program or the medium therefor which comprises the means for displaying the three-dimensional graphic display has advantages that visual studies and/or calculation of avidity can be made more conveniently, so that there is more facilitated a logical design on the three-dimensional structural level for obtaining a compound having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermomechanical stability, higher absorbency to a living body, and lower toxicity than those for known effectors of the dipeptidyl peptidase IV.

As the means capable of displaying the three-dimensional graphic display, there may be generally used a program that is made so that a means for inputting the three-dimensional structural coordinate of the molecule, a means for measuring visual representation of the coordinate on a computer screen, the distance between the represented atoms in the molecule, bond angles or the like, a means for addition or modification of the coordinate, and the like can be provided. Furthermore, there may be used a program that has been made so that a means for calculating the structure energy of the molecule based on the

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coordinate of the molecule, a means for calculating the free energy of bonding, and the ratio of bonding state number to non-bonding state number in consideration of solvent molecules such as water molecule can be provided. Examples of the program suitable for such purposes include Insight II, QUANTA and the like, which are computer programs commercially available from Accelrys Inc., and the present invention is not limited to these programs. Also, the above-mentioned programs can be introduced into a computer referred to as a work station supplied from Silicone Graphics Inc., SunMicro-Systems Ltd., or the like, and used.

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According to the crystal of dipeptidyl peptidase IV of the present invention, there can be exhibited excellent effects that the three-dimensional structural coordinate can be obtained as an information for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and that the crystal of a complex of the dipeptidyl peptidase IV and a known effector can be readily prepared. Also, according to the three-dimensional structural coordinate of the present invention, there is exhibited an excellent effect that the effector can be designed, identified, evaluated or searched. In addition, according to the method for obtaining a three-dimensional structural coordinate of the homolog protein of the dipeptidyl peptidase IV of the present invention, there is exhibited an excellent effect that the three-dimensional structural coordinate of the homolog protein of the dipeptidyl peptidase IV of which three-dimensional structure is unknown can be conveniently and rapidly provided. Furthermore, according to the method for

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obtaining a three-dimensional structure of a crystal of a complex of the dipeptidyl peptidase IV of the present invention and an effector of the dipeptidyl peptidase IV, there is exhibited an excellent effect that the method can provide a target for designing an effector useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermomechanical stability, and higher absorbency to a living body. Moreover, according to the method of the present invention for identifying a pharmacophore of the dipeptidyl peptidase IV and the effector of the dipeptidyl peptidase IV, there is exhibited an excellent effect that the method can provide a target for designing the effector useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermomechanical stability, and higher absorbency to a living body. According to the method of the present invention for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, there is exhibited an excellent effect that the method can logically and conveniently provide an effector useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermomechanical stability, and higher absorbency to a living body. According to the effector of the dipeptidyl peptidase IV of the present invention, there are exhibited excellent effects that the effector is capable of modifying immune response and capable of treating or preventing diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. Furthermore, according to the program and medium therefor of the present invention, there is exhibited an excellent effect that the method for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV can be performed more rapidly and conveniently.

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The present invention will be hereinafter more specifically explained by the following Examples, but the present invention is not intended to be limited by the Examples in any way. Unless otherwise indicated, the reaction conditions, procedures and the like can be referred to the instruction manual attached to the reagents used, *Molecular Cloning A Laboratory Manual*, third edition, Sambrook et al. [issued by Cold Spring Harbor Laboratory Press (2001)], and the like.

Example 1 Construction of Recombinant Baculovirus for Expression of Soluble Human Dipeptidyl Peptidase IV

20 (1) Cloning of Soluble Human Dipeptidyl Peptidase IV (shDPPIV) cDNA

Caco-2 cells [provided by American Type Culture Collection (ATCC)]

were cultured at 37°C using Dulbecco's Modified Eagle Medium (manufactured by Invitrogen) containing 20% by volume of inactivated fetal bovine serum (manufactured by Invitrogen; inactivated by incubation at 56°C for 30 minutes)

and 1% by volume of nonessential amino acid (manufactured by Invitrogen), in

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the presence of 5% by volume of CO₂.

Next, total RNA was extracted from the Caco-2 cells obtained.

Extraction of the total RNA was carried out using a product manufactured by Nippon Gene Co. Ltd. under the trade name of ISOGEN in accordance with the attached instruction manual. The obtained total RNA was used as a template for RT-nested PCR method described below.

In order to obtain a nucleic acid corresponding to a soluble human DPPIV from which the signal peptide sequence was removed (amino acid nos: 33-766 of SWISS-PROT Accession No: P27487), first, a cDNA fragment sequence of human DPPIV gene was amplified by RT-nested PCR method with total RNA of the Caco-2 as a template.

The thermal profile in the PCR is 30 cycles of reaction, in which one cycle comprises denaturation at 94°C for 30 seconds, annealing at 55°C for 30 seconds and polymerase extension reaction at 72°C for 1 minute.

The amplified DNA fragment was separated by agarose gel electrophoresis method, and a small fragment of the gel of the corresponding band portions was cut out. Thereafter, the DNA fragment was extracted from the obtained small fragments of the gel using a product manufactured by Bio 101 under the trade name of GENE CLEAN SPIN Kit, and purified. The obtained fragment was inserted into vector pCR2.1-TOPO contained in TOPO TA Cloning (registered trade mark) Kit manufactured by Invitrogen to construct pCR-shDPPIV.

In order to confirm whether or not the obtained cDNA fragment encodes the desired polypeptide, deletion mutants regarding the DNA fragment having various lengths were prepared, and a nucleotide sequence for the DNA fragment

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was determined as follows.

First, a DNA fragment having a size of 2.2 kbp obtained by double digestion of the pCR-shDPPIV with BamHI and EcoRI was inserted into a corresponding restriction site in pUC19 (manufactured by Takara Bio Inc.), to construct a plasmid pUshDPPIV. Various deletion plasmids were prepared using the plasmid pUshDPPIV by a conventional method.

The nucleotide sequence for the DNA fragment was determined using the obtained deletion plasmid or plasmid pCR-shDPPIV, and a product manufactured by Perkin-Elmer Cetus Inc. under the trade name of Taq DyeDeoxy Terminator Cycle Sequencing Kit and Model 373S sequencer manufactured by Applied Biosystems.

Also, the amino acid sequence of the polypeptide encoded by the abovementioned DNA fragment was determined on the basis of the nucleotide sequence.

The determined amino acid sequence was compared with the sequence for a full length DPPIV of human colon shown in SEQ ID NO: 2. As a result, it was confirmed that the corresponding regions (regions excluding the transmembrane region) were identical.

Thus, it was confirmed that the DNA fragment encodes the desired polypeptide shDPPIV, namely a polypeptide in which the transmembrane region (amino acid nos: 1-32 at N-terminal side) in the full-length human DPPIV was deleted and a polyhistidine peptide was added to the C-terminal side.

(2) Preparation of Recombinant Baculovirus

Plasmid pUshDPPIV was digested with a restriction enzyme to give a

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DNA fragment encoding shDPPIV gene. The obtained fragment was inserted into pAcGP67B (manufactured by BD PharMingen) to construct a baculovirus transfer vector pAcGP67B-shDPPIV.

Fifteen minutes before the transfection, Sf21 cells were washed twice with a TNM-FH medium comprising 10% by volume of fetal bovine serum. The Sf21 cells were then transferred to a well of a 6-well plate by 2.4×10^6 cells per well.

Furthermore, 2 to 5 µg of the baculovirus transfer vector and a 0.5 µg linear baculovirus DNA (trade name: BaculoGold virus DNA, manufactured by BD PharMingen) were mixed, and the mixture was allowed to stand at room temperature for 5 minutes. Next, 1 ml of Transfection Buffer B (manufactured by BD PharMingen) was added to the obtained mixture, and the mixture was thoroughly mixed to give a Transfection Buffer B/DNA mixture.

The medium in the wells of the 6-well plate and the cells that had not been adhered to the wells were removed, and 1 ml of Transfection Buffer A (manufactured by BD PharMingen) was added to each of the wells. The Transfection Buffer B/DNA mixture was gradually added dropwise to the wells of the 6-well plate, with gently stirring the 6-well plate. The cells were incubated at 28°C for 4 hours in the wells of the 6-well plate. Thereafter, the transfection buffer was removed, and 3 ml of TNM-FH medium containing 10% by volume of fetal bovine serum was added to the wells of the 6-well plate. The cells were cultured at 28°C in each of the wells of the 6-well plate for 5 days, and the culture supernatant was collected. The culture supernatant was used for amplification of virus using Sf21 cells to give a virus stock solution.

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Example 2 Preparation and Crystallization of shDPPIV

(1) Expression of shDPPIV in Insect Cells

Sf21 cells were cultured using a serum free medium EX-CELL 400 (manufactured by JRH Biosciences) and T flask, and Tn5 cells (provided by Invitrogen) were cultured using a serum free medium EX-CELL 401 (manufactured by JRH Biosciences) and a T flask, at 28°C, respectively. At the time when the proliferation of the cells reached 70% confluent, the old medium was removed, and a fresh medium was added at 40 ml per one 225-cm² flask. Then, 1.5 ml of virus stock solution after amplification for three times (having multiplicity of infection (MOI) of about 2) was added to the cells to infect the cells, and the cells were incubated at 28°C for 4 days. The culture supernatant four days after the infection was collected and stored at -20°C. The culture supernatant was used for the purification of shDPPIV protein as described below.

15 (2) Purification of shDPPIV Protein

In each step for the purification of shDPPIV, the activity of DPPIV was measured by incubating a 0.1 ml reaction mixture containing a 1.5 mM substrate [manufactured by Peptide Institute, Gly-Pro-paranitroanilide (pNA)], 71 mM Gly-NaOH (pH 8.7) and the DPPIV, and detecting the liberated pNA.

Meanwhile, the reaction mixture was incubated at 37°C for 10 minutes. During the incubation, the absorbance at 405 nm was monitored.

Also, the protein concentration was quantified by using a product manufactured by Bio-Rad Laboratories, Inc. under the trade name of DC protein Assay Kit II.

The purity of the protein was confirmed by subjecting a protein sample

in each step to SDS-PAGE using 7.5% polyacrylamide gel according to the method by Laemmli et al.

The culture supernatant stored at -20°C in the above-mentioned (1) was melted at 4°C and filtered with a bottle top filter (manufactured by Becton, Dickinson and Company) or with 0.45 µm filter (KURABO INDUSTRIES LTD.) to remove insoluble materials. The supernatant after the filtration was concentrated to an about tenth volume by using a concentrator Vivaflow 50 (manufactured by Sartorius AG) or Amicon stirrer cell model 8400 (manufactured by Millipore Corporation) to give a concentrated solution.

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The obtained concentrated solution was dialyzed against buffer A (20 mM HEPES-NaOH, 0.5 M NaCl, pH 8.0) at 4°C overnight, and applied to a nickel column [one in which nickel was immobilized to HiTrap Chelating column (trade name, manufactured by Amersham-Pharmacia) (5 ml × 2)] equilibrated with buffer A. The column was washed with 10 column volumes of buffer A, and then with buffer A containing 50 mM imidazole. The elution of the fraction containing shDPPIV was carried out by a linear gradient of 50 to 500 mM imidazole. The fraction found to have DPPIV activity was collected, and dialyzed overnight at 4°C against buffer B (20 mM HEPES-NaOH, pH 8.0, 50 mM NaCl). After the dialysis, the sample was purified by using an anion exchange column [manufactured by Amersham-Pharmacia under the trade name: Resource Q (6 ml)] equilibrated with buffer B. The column was washed with buffer B, and thereafter shDPPIV was eluted by a linear gradient of 15 column volumes of 50 to 500 mM NaCl. The fractions found to have DPPIV activity were collected, and used as a purified preparation.

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(3) Preparation of Protein Sample for Crystallization

The shDPPIV purification sample (9 ml) obtained in the above (2) was concentrated using a product manufactured by Millipore Corporation under the trade name of Centricon 10 until the protein concentration reached 10 mg/ml.

The obtained product was used as a protein sample for crystallization.

The protein sample for crystallization was stored at 4°C.

A precipitation agent solution containing 0.18 M glycine-NaOH (pH 9.5), 0.18 M sodium sulfate and 18% by weight of PEG4000, and a 10 mg/ml dipeptidyl peptidase IV solution were mixed, and thereafter, a drop of the obtained mixed solution was placed on a product under the trade name of Cryschem Plate (manufactured by Hampton Research). The above-mentioned precipitation solution was allowed to stand at 20°C as a reservoir solution to allow crystallization.

15 (4) Crystallization of shDPPIV

The crystallization of shDPPIV was carried out by a sitting-drop method, which is one of vapor diffusion methods.

The formation of crystal was observed with the passage of time using a stereoscopic microscope. As a result, after about two weeks, a large crystal having a maximum size of 500 μ m \times 300 μ m \times 100 μ m was obtained. The crystal is also referred to as a native crystal. The microphotograph of the obtained crystal is shown in Figure 1. In Figure 1, the visual field is 4000 μ m \times 3000 μ m.

Example 3 Three-Dimensional Structural Analysis of Crystals

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(1) X-ray Diffraction

The crystal obtained in Example 2 mentioned above was soaked in a cryoprotecting buffer [composition: 0.18 M glycine-NaOH (pH 9.5), 19% by weight of PEG4000, 0.18 M sodium acetate, 15% glycerol], and immediately thereafter the mixture was placed under nitrogen gas stream (100 K) to rapidly freeze the mixture.

The X-ray diffraction intensity data of the above crystal were collected up to the resolution of 3.0Å using a product manufactured by Rigaku International Corporation under the trade name of R-AXIS IV in nitrogen gas stream (100 K), and converted to the structure factor using a program MOSFLM (Version 6.11). A photograph of the diffraction pattern is shown in Figure 2.

From the obtained diffraction intensity data, it was determined that the crystal form to which the crystal belongs was orthorhombic, that the space group was $P2_12_12_1$, and the lattice constants were $a = 118.0 \pm 5.0$ Å, $|b| = 125.9 \pm 5.0$ Å and $|c| = 136.8 \pm 5.0$ Å.

(2) Multiple Isomorphous Replacement Method

In order to derive an electron density map, multiple isomorphous replacement method was carried out. The crystal obtained in Example 2 was soaked for 3 days and 4 days in a crystallization solution prepared by dissolving mercury chloride until being saturated, to give two different kinds of isomorphous replacement crystals containing mercury atoms in the crystals. The X-ray diffraction intensity data were collected in the same manner as those for the native crystals.

In the determination of the phase in the structural analysis, CCP4

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(Collaborative Computational Project, Number 4, 1994. "The CCP4 Suite: Programs for Protein Crystallography," *Acta Cryst.* D50, 760-763) program was used.

First, Fourier transform calculation utilizing the difference between the diffraction intensity obtained from the two kinds of isomorphous replacement crystals of mercury and the diffraction intensity obtained from the native crystal was performed using MLPHERE contained in the CCP program package. The position of each mercury atom in the unit cell of the real space was determined by investigating large peaks provided by heavy atoms (mercury) in the obtained Patterson's diagram. The phase of the crystal structure factor of the native crystals was determined by using the obtained position coordinate of mercury atoms. Furthermore, in order to determine the coordinate of each mercury atom more accurately using DM and SOLOMON contained in the CCP program package, refinement was carried out using three crystal structure factors of the native crystals and of the two kinds of mercury isomorphous replacement crystals.

An electron density map of the crystals of the dipeptidyl peptidase IV in real space was obtained using the phase of the crystal structure factor of the native crystals calculated from the refined coordinates of the mercury atoms. Furthermore, the electron density map was improved by carrying out smoothening and histogram matching of the electron density map in a solvent region, to obtain an electron density map critical for molecular modeling.

(3) Molecular Modeling

The sites corresponding to the amino acid residues of the dipeptidyl

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peptidase IV were identified on the electron density map by using QUANTA (manufactured by Accelrys, Inc.), to build molecular models.

As expected from the lattice constants, there were two molecules of the dipeptidyl peptidase IV in an asymmetry unit, and a model was built for each of the molecules. The refinement of the obtained molecular model was carried out using CNX (manufactured by Accelrys, Inc.), and the molecular model was adjusted again using the QUANTA for the obtained improved electron density map. The procedures were repeated to build a more accurate molecular model. In the refinement of the final coordinate, diffraction intensity data measured again were used after OSMIC confocal mirror (manufactured by Rigaku International Corporation) had been introduced into R-AXIS IV (trade name, manufactured by Rigaku International Corporation).

As a result, the resolution was improved from the previous 3.0Å to 2.6Å. Furthermore, 273 molecules of bound water and 5 molecules of N-acetyl glucosamine residues per molecule of the dipeptidyl peptidase IV were identified in an asymmetric unit. R factor, which is an index for accuracy of the obtained molecular model, was 24.89%, and a free R factor, which independently was not taken into account of the calculation of refinement at the step of refinement, was 30.15%. During the procedure, the deviation of the interatomic bond distance (rms-deviation) and the bond angle from the ideal state of the three-dimensional structure were 0.006Å and 1.305°, respectively. The stereogram of the three-dimensional structure model of the crystals is shown in Figure 3, and the coordinate is shown in Figure 4. The present coordinate data were registered in PDB (Brookhaven Protein Data Bank) [PDB Code No: 1J2E, RSCB code No: 005544].

Here, as to those regions which did not take a regular structure in the crystals (in the disordered state), namely, the region from Asp 38 to that closer to the N-terminal side thereof, and the region for the tagged peptide (polyhistidine peptide) of the C-terminal side, the molecular model could not be built.

Furthermore, a part of the side chains projected to the surface of the molecules did not take a regular structure. However, these residues were not portions that play an important role for the function of enzymes.

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In the three-dimensional structure of the dipeptidyl peptidase IV, which has been clarified by the Examples, it has been revealed that the amino acid residue involved in the activity deduced by various experiments for the dipeptidyl peptidase IV, namely, Ser 630, Asp 708 and His 740, form hydrogen bonds between the $O_{\delta 2}$ atom of Asp 708 and $N_{\delta 1}$ atom of His 740, and with the $N_{\epsilon 2}$ atom of His 740 and O_{γ} atom of Ser 630, even the residues locate in distant locations on the primary sequence. Therefore, for the structural coordinate of Figure 4 and the three-dimensional structure model defined by the structural coordinate, it is suggested that the regions characterized by Ser 630, Asp 708 and His 740, and the whole or a part of amino acid residues that are located in the vicinity of Ser 630, Asp 708 and His 740 play an important role on the exhibition of the activity for the dipeptidyl peptidase IV and binding or interaction of the dipeptidyl peptidase IV with the effector, and that the compound matching the three-dimensional structure of the regions affect the activity for the dipeptidyl peptidase IV.

The present invention may be embodied in other various forms without departing from the spirit or essential characteristics thereof. The present

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embodiment is therefore to be considered in all respects as illustrative and not restrictive, the scope of the invention being indicated by the appended claims rather than by the foregoing description and all changes which come within the meaning and range of equivalency of the claims are therefore intended to be embraced therein.

INDUSTRIAL APPLICABILITY

According to the crystal of the dipeptidyl peptidase IV of the present invention, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like can be obtained. Also, according to the three-dimensional structure coordinate, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like can be obtained. Further, according to the method of the present invention for obtaining a threedimensional structure coordinate of a homolog protein of a dipeptidyl peptidase IV, the refinement of the three-dimensional structure coordinate of the homolog protein of the dipeptidyl peptidase IV can be more conveniently carried out. Moreover, according to the method of the present invention for obtaining a threedimensional structure coordinate of a crystal of a complex of a dipeptidyl

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peptidase IV with an effector of the dipeptidyl peptidase IV, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, which is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency to a living body, and which can favorably act on the dipeptidyl peptidase IV can be obtained. Also, according to the method for identifying a pharmacophore of a dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, which is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency to a living body, and which can favorably act on the dipeptidyl peptidase IV can be obtained. Further, according to the method of the present invention for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV. which is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency to a living body,

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and which can favorably act on the dipeptidyl peptidase IV can be logically and conveniently obtained. In addition, the effector of the dipeptidyl peptidase IV of the present invention is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. Further, according to the program or the medium therefor of the present invention, the design, identification, evaluation and search for an effector of a dipeptidyl peptidase IV can be carried out rapidly and conveniently. Therefore, the present invention can be utilized in modulation of immune response and the treatment or prevention for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like.

CLAIMS

- 1. A crystal of a dipeptidyl peptidase IV, having characteristics sufficient to ensure a resolution capable of analyzing its three-dimensional structure up to the side chain level by X-ray crystallographic structural analysis.
- 2. The crystal according to claim 1, wherein the dipeptidyl peptidase IV is a soluble polypeptide comprising a region located at extramembrane in a full-length human dipeptidyl peptidase IV.

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3. The crystal according to claim 1 or 2, wherein the dipeptidyl peptidase IV is a polypeptide having an amino acid sequence in which a transmembrane region is deleted from the amino acid sequence of SEQ ID NO: 2, and a tag peptide is optionally added to a C-terminal side or N-terminal side thereof.

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4. The crystal according to any one of claims 1 to 3, wherein the crystal has a space group of $P2_12_12_1$, and a lattice constant of the unit cell of $|a| = 118.0 \pm 5.0$ Å, $|b| = 125.9 \pm 5.0$ Å, $|c| = 136.8 \pm 5.0$ Å, and $\alpha = \beta = \gamma = 90^{\circ}$, and is orthorhombic.

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- 5. The crystal according to any one of claims 1 to 4, wherein the crystal has the structural coordinate shown in Figure 4.
- 6. The crystal according to any one of claims 1 to 4, wherein the crystal has
 25 a structural coordinate different from the structural coordinate as shown in

Figure 4 via fluctuation of a protein.

- 7. A three-dimensional structural coordinate of a dipeptidyl peptidase IV, comprising the structural coordinate shown in Figure 4.
- 8. A three-dimensional structural coordinate of a dipeptidyl peptidase IV, comprising a structural coordinate different from the structural coordinate as shown in Figure 4 via fluctuation of a protein.
- 9. The three-dimensional structural coordinate according to claim 8, wherein the fluctuation of a protein is a state that is caused by molecular oscillation or temperature, and exhibits an activity for the dipeptidyl peptidase IV in a living body.
- 10. The three-dimensional structural coordinate according to any one of claims 7 to 9, wherein the dipeptidyl peptidase IV is a soluble polypeptide comprising a region located at extramembrane in a full-length human dipeptidyl peptidase IV.
- 20 11. The three-dimensional structural coordinate according to any one of claims 7 to 10, wherein the dipeptidyl peptidase IV is a polypeptide having an amino acid sequence in which a transmembrane region is deleted from the amino acid sequence of SEQ ID NO: 2, and a tag peptide is optionally added of to a Cterminal side or N-terminal side thereof.

- 12. A three-dimensional structural coordinate of a region in a dipeptidyl peptidase IV, comprising the three-dimensional structural coordinate of the region selected from the group consisting of the following (a) to (d):
- (a) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of the amino acid residues located in the adjacent area of each of the Ser 630, Asp 708 and His 740 in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate;
- (b) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of the amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of amino acids in the group of the amino acid residues
 located in the adjacent area of each of Ser 630, Asp 708 and His 740, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate,
- (c) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics

 20 physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of the amino acid residues located adjacent area of said group of the amino acid residues in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate; and

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(d) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of the amino acids in the group of the amino acid residues located in the adjacent area of said group of the amino acids, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate,

wherein the region in the dipeptidyl peptidase IV is a region involved in binding or interaction between the dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV.

- 13. The three-dimensional coordinate according to claim 12, wherein the physicochemical characteristic is selected from the group consisting of features in shape of a three-dimensional structure, hydrophobicity, electric charge and pK.
- 14. A method for obtaining a three-dimensional coordinate of a homolog protein of a dipeptidyl peptidase IV, characterized in refining an electron density map of the homolog protein of the dipeptidyl peptidase IV comprising the amino acid sequence of SEQ ID NO: 2, based on all and/or a part of the three-dimensional coordinate of any one of claims 7 to 13, to give a three-dimensional structural coordinate.

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- 15. A method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV characterized in using all and/or a part of the three-dimensional structural coordinate of any one of claims 7 to 13, to give a three-dimensional structural coordinate.
- 16. A method for identifying pharmacophore of an effector of the dipeptidyl peptidase IV, characterized in identifying the pharmacophore based on all and/or a part of the three-dimensional structural coordinate of any one of claims 7 to 13, and the steric conformation of the effector of the dipeptidyl peptidase IV.
- 17. A method for designing, identifying, evaluating or searching an effector of a dipeptidyl peptidase IV, characterized in designing, identifying, evaluating or searching a compound capable of acting on the dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate of any one of claims 7 to 13.
- 18. The method according to claim 17, wherein the method for designing, identifying, evaluating or searching an effector comprises the steps of:
- 20 (i) identifying a region to be targeted for binding or interaction with the effector in a dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate according to any one of claims 7 to 13 and the steric conformation of the effector of the dipeptidyl peptidase IV;
- 25 (ii) identifying atoms or atomic groups capable of generating in the above

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region at least one intermolecular interaction selected from the group consisting of covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction and hydrophobic interaction, with the atoms or atomic groups existing in a candidate compound; and

- (iii) designing a compound based on the information of the above step (i) and/or (ii).
- 19. The method according to claim 18, wherein the method further comprises

 the steps of:

detecting an interaction between the dipeptidyl peptidase IV and the designed, identified, evaluated or searched candidate compound, wherein when an interaction is detected, the candidate compound is identified as a compound capable of binding to the dipeptidyl peptidase IV, based on a degree of the interaction as an index.

20. The method according to claim 18 or 19, wherein the method further comprises the steps of:

contacting the dipeptidyl peptidase IV with the designed, identified, evaluated or searched candidate compound and measuring an activity of the dipeptidyl peptidase IV, wherein when an activity increases or decreases, the designed, identified, evaluated or searched candidate compound is identified as a compound having enhancing action or inhibitory action on the activity of the dipeptidyl peptidase IV, based on a degree of the increase or decrease as an index.

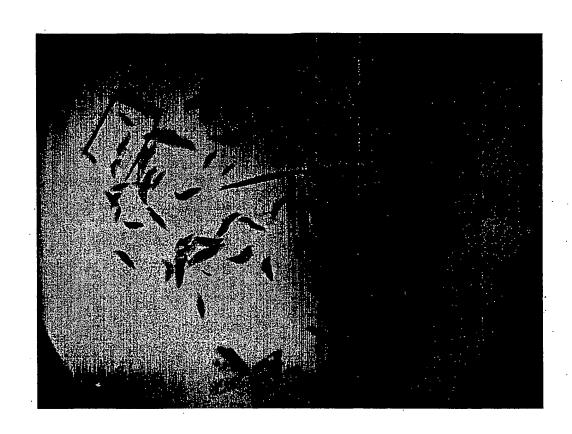
- 21. An effector of the dipeptidyl peptidase IV obtainable by the method of any one of claims 17 to 20.
- 5 22. A program and a medium therefor for use of the three-dimensional structural coordinate of any one of claims 7 to 13, wherein all and/or a part of the three-dimensional structural coordinate of any one of claims 7 to 13 is recorded.
- 23. The program and the medium according to claim 22, comprising a means for identifying, searching, evaluating or designing a compound capable of binding to the dipeptidyl peptidase IV or a compound having an enhancing action or inhibitory action on the activity for the dipeptidyl peptidase IV.
- 24. The program and the medium according to claim 23, further comprising a means for displaying a three-dimensional graphic display of a molecule.

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FIG. 1



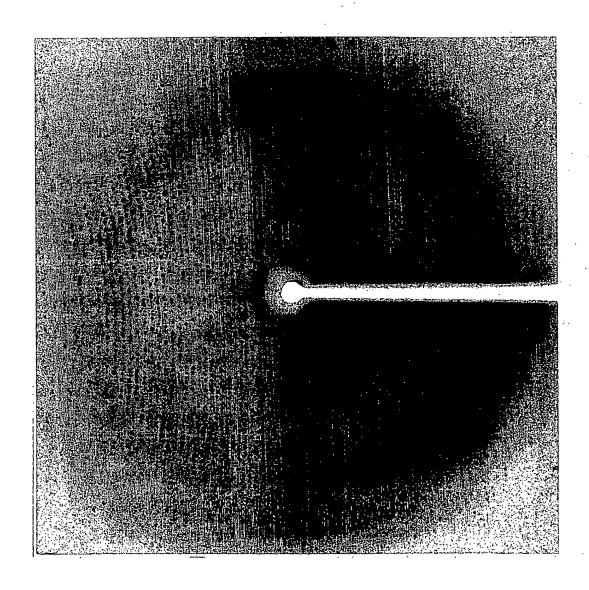
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FIG. 2



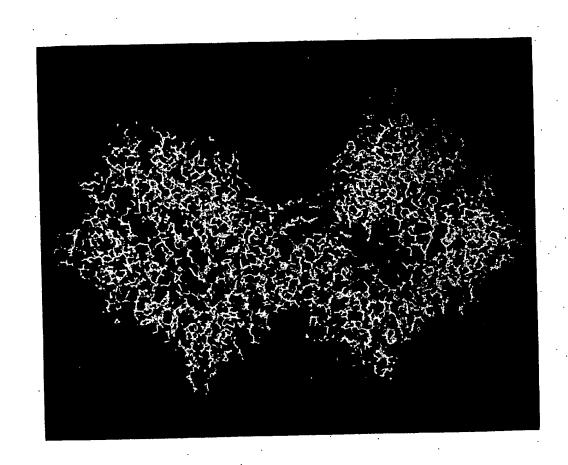
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FIG. 3



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FIG. 4-1

ATOM 1 CB ASP 38 44.493 31.885 58.927 1.00 42.46 A C ATOM 2 CG ASP 38 44.146 32.095 57.467 1.00 42.00 A C ATOM 3 0D1 ASP 38 44.366 31.171 56.655 1.00 42.05 A C ATOM 4 0D2 ASP 38 44.864 31.171 56.655 1.00 42.55 A 0 ATOM 5 C ASP 38 45.876 29.805 58.634 1.00 41.68 A C ATOM 6 O ASP 38 46.980 30.272 58.778 1.00 42.20 A O ATOM 7 N ASP 38 44.6590 30.272 58.778 1.00 42.28 A N ATOM 8 CA ASP 38 44.6590 30.272 58.778 1.00 42.88 A N ATOM 8 CA ASP 38 44.659 30.404 59.296 1.00 42.51 A C ATOM 10 CA SER 39 46.775 28.013 57.241 1.00 39.98 A C ATOM 11 CB SER 39 46.577 28.013 57.241 1.00 39.98 A C ATOM 11 CB SER 39 46.576 28.711 57.905 1.00 40.69 A N ATOM 12 0G SER 39 46.906 28.343 55.763 1.00 41.11 A O ATOM 14 O SER 39 45.410 26.079 56.703 1.00 41.11 A O ATOM 14 O SER 39 45.400 28.343 55.763 1.00 39.60 A C ATOM 15 N ARG 40 46.093 29.190 55.217 1.00 38.12 A N ATOM 16 CA ARG 40 46.093 29.190 55.217 1.00 38.12 A N ATOM 16 CA ARG 40 46.993 29.190 55.217 1.00 38.12 A N ATOM 17 CB ARG 40 46.5082 30.558 53.310 1.00 37.02 A C ATOM 17 CB ARG 40 44.683 29.984 53.404 1.00 35.97 A C ATOM 19 CD ARG 40 42.688 31.095 58.310 1.00 35.97 A C ATOM 19 CD ARG 40 42.688 31.095 58.311 1.00 35.57 A C ATOM 22 NFI ARG 40 42.2774 32.134 54.161 1.00 35.577 A N ATOM 22 NFI ARG 40 42.2774 32.134 54.161 1.00 35.577 A C ATOM 22 NFI ARG 40 42.297 33.276 54.125 1.00 35.554 A N ATOM 22 NFI ARG 40 42.297 33.276 54.125 1.00 35.554 A N ATOM 22 NFI ARG 40 42.297 33.276 54.125 1.00 35.557 A C ATOM 22 NFI ARG 40 42.293 34.167 55.097 1.00 34.68 A N ATOM 22 NFI ARG 40 42.293 34.167 55.097 1.00 35.54 A N ATOM 22 NFI ARG 40 42.293 34.167 55.097 1.00 35.55 A C C ATOM 32 NFI ARG 40 42.293 34.167 55.597 1.00 35.55 A C C ATOM 32 NFI ARG 40 42.293 34.167 55.097 1.00 35.55 A C C ATOM 32 NFI ARG 40 42.293 34.167 55.097 1.00 35.54 A N ATOM 24 C ARG 40 44.288 31.095 1.00 35.97 A C ATOM 35 N THR 42 50.100 33.505 51.954 1.00 35.73 A C ATOM 37 C B THR 42 50.506 35.139 53.000 1.00 33.41 A C ATOM 37 C B THR 42 50.506 35.139 53.000 1.00 33.41 A C ATOM 37 C B THR 42 50.506 35.139 53.000 1		Th	ree-	-dime	nsional	structural	coordin	ate of o	dipeptidyl	peptidase	IV
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ATOM 38 OG1 THR 42 52. 234 34. 843 52. 725 1. 00 30. 79 A 0 ATOM 39 CG2 THR 42 50. 501 34. 622 54. 386 1. 00 30. 12 A C ATOM 40 C THR 42 50. 389 34. 971 50. 558 1. 00 28. 34 A C ATOM 41 0 THR 42 50. 977 34. 220 49. 782 1. 00 27. 76 A 0 ATOM 42 N TYR 43 50. 058 36. 217 50. 234 1. 00 27. 55 A N ATOM 43 CA TYR 43 50. 465 36. 782 48. 954 1. 00 25. 72 A C ATOM 44 CB TYR 43 49. 615 38. 006 48. 623 1. 00 26. 01 A C ATOM 45 CG TYR 43 49. 922 38. 625 47. 280 1. 00 26. 92 A C ATOM 46 CD1 TYR 43 50. 977 39. 527 47. 130 1. 00 26. 68 A C ATOM 47 CE1 TYR 43 51. 253 40. 113 45. 895 1. 00 27. 02 A C											
ATOM											
ATOM 40 C THR 42 50.389 34.971 50.558 1.00 28.34 A C ATOM 41 0 THR 42 50.977 34.220 49.782 1.00 27.76 A 0 ATOM 42 N TYR 43 50.058 36.217 50.234 1.00 27.55 A N ATOM 43 CA TYR 43 50.465 36.782 48.954 1.00 25.72 A C ATOM 44 CB TYR 43 49.615 38.006 48.623 1.00 26.01 A C ATOM 45 CG TYR 43 49.922 38.625 47.280 1.00 26.92 A C ATOM 46 CD1 TYR 43 50.977 39.527 47.130 1.00 26.68 A C ATOM 47 CE1 TYR 43 51.253 40.113 45.895 1.00 27.02 A C										_	
ATOM 41 0 THR 42 50.977 34.220 49.782 1.00 27.76 A 0 ATOM 42 N TYR 43 50.058 36.217 50.234 1.00 27.55 A N ATOM 43 CA TYR 43 50.465 36.782 48.954 1.00 25.72 A C ATOM 44 CB TYR 43 49.615 38.006 48.623 1.00 26.01 A C ATOM 45 CG TYR 43 49.922 38.625 47.280 1.00 26.92 A C ATOM 46 CD1 TYR 43 50.977 39.527 47.130 1.00 26.68 A C ATOM 47 CE1 TYR 43 51.253 40.113 45.895 1.00 27.02 A C											č
ATOM 42 N TYR 43 50.058 36.217 50.234 1.00 27.55 A N ATOM 43 CA TYR 43 50.465 36.782 48.954 1.00 25.72 A C ATOM 44 CB TYR 43 49.615 38.006 48.623 1.00 26.01 A C ATOM 45 CG TYR 43 49.922 38.625 47.280 1.00 26.92 A C ATOM 46 CD1 TYR 43 50.977 39.527 47.130 1.00 26.68 A C ATOM 47 CE1 TYR 43 51.253 40.113 45.895 1.00 27.02 A C											
ATOM 43 CA TYR 43 50.465 36.782 48.954 1.00 25.72 A C ATOM 44 CB TYR 43 49.615 38.006 48.623 1.00 26.01 A C ATOM 45 CG TYR 43 49.922 38.625 47.280 1.00 26.92 A C ATOM 46 CD1 TYR 43 50.977 39.527 47.130 1.00 26.68 A C ATOM 47 CE1 TYR 43 51.253 40.113 45.895 1.00 27.02 A C											
ATOM 44 CB TYR 43 49.615 38.006 48.623 1.00 26.01 A C ATOM 45 CG TYR 43 49.922 38.625 47.280 1.00 26.92 A C ATOM 46 CD1 TYR 43 50.977 39.527 47.130 1.00 26.68 A C ATOM 47 CE1 TYR 43 51.253 40.113 45.895 1.00 27.02 A C				TYR					1.00 25.7		Ċ
ATOM 45 CG TYR 43 49.922 38.625 47.280 1.00 26.92 A C ATOM 46 CD1 TYR 43 50.977 39.527 47.130 1.00 26.68 A C ATOM 47 CE1 TYR 43 51.253 40.113 45.895 1.00 27.02 A C				TYR	43						Č
ATOM 46 CD1 TYR 43 50.977 39.527 47.130 1.00 26.68 A C ATOM 47 CE1 TYR 43 51.253 40.113 45.895 1.00 27.02 A C						49.922	38. 625				Ċ
ATOM 47 CE1 TYR 43 51.253 40.113 45.895 1.00 27.02 A C									1.00 26.6		C
ATOM 48 CD2 TYR 43 49.152 38.315 46.158 1.00 26.40 A C						51.253	40.113	45.895	1.00 27.0	2 A	С
	ATOM	48	CD2	TYR	43	49. 152	38. 315	46. 158	1.00 26.4	0 A	С

				(Continued)
			FIG. 4-2	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	49 CE2 TYR 50 CZ TYR 51 OH TYR 52 C TYR 53 O TYR 54 N THR 55 CA THR 56 CB THR 57 OG1 THR 58 CG2 THR 60 O THR 61 N LEU 62 CA LEU 63 CB LEU 64 CG LEU 65 CD1 LEU 66 CD2 LEU 67 C LEU 67 C LEU 68 O LEU 69 N THR 70 CA THR	43 43 43 43 44 44 44 44 45 45 45 45 45 46 46	49. 424 38. 891 44. 919 1. 00 25. 89 50. 473 39. 790 44. 796 1. 00 25. 91 50. 741 40. 370 43. 579 1. 00 25. 09 51. 933 37. 165 49. 160 1. 00 24. 97 52. 251 38. 049 49. 955 1. 00 23. 33 52. 818 36. 482 48. 444 1. 00 24. 06 54. 255 36. 685 48. 580 1. 00 25. 90 54. 960 35. 336 48. 547 1. 00 25. 86 54. 696 34. 709 47. 285 1. 00 28. 12 54. 439 34. 436 49. 655 1. 00 22. 61 54. 917 37. 576 47. 530 1. 00 27. 35 54. 296 37. 956 46. 535 1. 00 29. 11 56. 191 37. 894 47. 765 1. 00 27. 39 56. 978 38. 722 46. 853 1. 00 26. 43 58. 377 38. 954 47. 425 1. 00 26. 21 58. 734 41. 263 46.	A C C A O C A C C C A C C C A C C C A C C C A C C C A C C C A C C C A C C C A C C C A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	71 CB THR 72 OG1 THR 73 CG2 THR 74 C THR 75 O THR 76 N ASP 77 CA ASP 78 CB ASP	46 46 46 46 47 47	57. 838 34. 559 44. 407 1. 00 26. 87 59. 150 34. 495 44. 966 1. 00 31. 74 57. 833 33. 793 43. 110 1. 00 28. 08 56. 076 36. 091 43. 517 1. 00 26. 96 55. 965 36. 094 42. 289 1. 00 25. 36 55. 035 36. 126 44. 346 1. 00 27. 72 53. 659 36. 199 43. 858 1. 00 29. 74 52. 670 36. 173 45. 026 1. 00 30. 90	A C A O A C A C A O A N A C A C A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	79 CG ASP 80 OD1 ASP 81 OD2 ASP 82 C ASP 83 O ASP 84 N TYR 85 CA TYR 86 CB TYR 87 CG TYR 88 CD1 TYR 89 CE1 TYR 90 CD2 TYR 91 CE2 TYR 92 CZ TYR 93 OH TYR	47 47 47 48 48 48 48 48 48 48 48 48	51. 778 34. 595 46. 553 1. 00 32. 28 52. 490 33. 845 44. 617 1. 00 30. 71 53. 477 37. 482 43. 073 1. 00 28. 87 52. 918 37. 478 41. 979 1. 00 29. 50 53. 945 38. 581 43. 648 1. 00 28. 54 53. 859 39. 878 42. 994 1. 00 29. 04 54. 191 40. 991 43. 996 1. 00 27. 50 54. 448 42. 333 43. 354 1. 00 25. 16 53. 460 42. 971 42. 609 1. 00 23. 19 53. 703 44. 184 41. 982 1. 00 24. 84 55. 694 42. 946 43. 461 1. 00 25. 89 55. 956 44. 165 42. 838 1. 00 26. 76 54. 955 44. 779 42. 096 1. 00 27. 28 55. 208 45. 977 41. 463 1. 00 25. 97	A
ATOM ATOM ATOM ATOM	94 C TYR 95 O TYR 96 N LEU 97 CA LEU	48 48 49 49	54. 820 39. 953 41. 796 1. 00 28. 80 54. 445 40. 401 40. 714 1. 00 28. 24 56. 054 39. 499 41. 988 1. 00 29. 41 57. 046 39. 552 40. 918 1. 00 30. 39	A C A O A N A C

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				F I G. 4 - 3	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	98 99 100 101 102 103 104 105 106 107 108	CB LEU CG LEU CD1 LEU CD2 LEU C LEU O LEU N LYS CA LYS CB LYS CG LYS CD LYS	49 49 49 49 49 50 50 50	56. 804 38. 606 39. 752 1. 00 30. 71 A 57. 147 38. 919 38. 614 1. 00 30. 14 A 56. 198 37. 459 40. 024 1. 00 32. 51 A 55. 959 36. 491 38. 971 1. 00 33. 54 A 56. 289 35. 098 39. 485 1. 00 33. 30 A 57. 763 34. 940 39. 790 1. 00 33. 89 A	A C A C A C A C A O A N A C
ATOM ATOM ATOM ATOM ATOM ATOM	109 110 111 112 113 114	CE LYS NZ LYS C LYS O LYS N ASN CA ASN	50 50 50 50 51	60. 071 34. 945 38. 778 1. 00 38. 12 4 60. 859 35. 028 37. 515 1. 00 39. 27 4 54. 572 36. 517 38. 361 1. 00 34. 93 4 54. 272 35. 719 37. 478 1. 00 35. 13 4 53. 731 37. 436 38. 822 1. 00 36. 66 4 52. 379 37. 569 38. 294 1. 00 38. 39 4	A C A N A C A O A N A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	115 116 117 118 119 120 121	CB ASN CG ASN OD1 ASN ND2 ASN C ASN O ASN N THR	51 51 51 51 51 51 52	53. 407 38. 968 36. 436 1. 00 44. 75 53. 212 40. 131 36. 801 1. 00 46. 38	0 /
ATOM ATOM ATOM ATOM ATOM ATOM	122 123 124 125 126 127	CA THR CB THR OG1 THR CG2 THR C THR O THR	52 52 52 52 52 52 52	50. 942 34. 451 39. 926 1. 00 35. 44 A 51. 297 33. 888 41. 298 1. 00 35. 57 A 52. 646 33. 415 41. 272 1. 00 38. 62 A 50. 367 32. 750 41. 666 1. 00 35. 25 A 49. 431 34. 686 39. 869 1. 00 35. 17 A 48. 699 33. 889 39. 276 1. 00 36. 44 A	A C A C A O A C A C A O
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	128 129 130 131 132 133 134	N TYR CA TYR CB TYR CG TYR CD1 TYR CE1 TYR CD2 TYR	53 53 53 53 53 53	47. 535 36. 081 40. 487 1. 00 33. 46 47. 084 36. 407 41. 903 1. 00 32. 64 47. 399 35. 293 42. 861 1. 00 33. 83 48. 341 35. 462 43. 872 1. 00 34. 11 48. 657 34. 425 44. 741 1. 00 34. 24 46. 775 34. 050 42. 741 1. 00 36. 17 47. 48	A N A C A C A C A C A C A C A C A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	135 136 137 138 139 140 141	CE2 TYR CZ TYR OH TYR C TYR O TYR N ARG CA ARG	53 53 53 53 53 54 54	48. 026 33. 199 44. 601 1. 00 35. 74 48. 343 32. 170 45. 453 1. 00 35. 79 47. 266 37. 248 39. 548 1. 00 33. 40	
ATOM ATOM ATOM ATOM ATOM	141 142 143 144 145 146	CB ARG CG ARG CD ARG NE ARG CZ ARG	54 54 54 54 54	46. 993 37. 387 35. 972 1. 00 35. 72 46. 887 38. 373 34. 821 1. 00 39. 96 47. 675 37. 880 33. 613 1. 00 43. 22 47. 651 38. 831 32. 506 1. 00 46. 7	A C A C A C A N A C

	٠.		(Continued)
ATOM ATOM ATOM ATOM ATOM	147 NH1 ARG 148 NH2 ARG 149 C ARG 150 O ARG 151 N LEU 152 CA LEU	54 54 54 54 55 55	FIG. 4 - 4 45. 451 38. 416 31. 968 1. 00 49. 25
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	153 CB LEU 154 CG LEU 155 CD1 LEU 156 CD2 LEU 157 C LEU 158 O LEU 159 N LYS	55 55 55 55 55 55 56 56	43. 792 41. 892 37. 123 1. 00 29. 74 A C 44. 042 42. 344 38. 557 1. 00 32. 26 A C 44. 245 43. 847 38. 571 1. 00 31. 83 A C 42. 857 41. 967 39. 448 1. 00 33. 66 A C 43. 298 40. 271 35. 322 1. 00 32. 61 A C 44. 004 40. 769 34. 441 1. 00 33. 62 A O 42. 189 39. 593 35. 050 1. 00 31. 32 A N 41. 733 39. 462 33. 673 1. 00 31. 42 A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	161 CB LYS 162 CG LYS 163 CD LYS 164 CE LYS 165 NZ LYS 166 C LYS 167 O LYS	56 56 56 56 56 56	40. 584 38. 453 33. 564 1.00 33. 54 A C 40. 978 36. 997 33. 733 1.00 34. 84 A C 41. 746 36. 484 32. 530 1.00 38. 85 A C 42. 120 35. 009 32. 698 1.00 40. 95 A C 43. 117 34. 537 31. 685 1.00 43. 33 A N 41. 240 40. 844 33. 252 1.00 30. 03 A C 40. 839 41. 648 34. 088 1. 00 28. 24 A 0 41. 286 41. 120 31. 956 1. 00 30. 20 A N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	168 N LEU 169 CA LEU 170 CB LEU 171 CG LEU 172 CD1 LEU 173 CD2 LEU 174 C LEU 175 O LEU	57 57 57 57 57 57 57 57	40.836 42.404 31.437 1.00 29.43 A C 42.022 43.233 30.934 1.00 30.04 A C 43.230 43.474 31.844 1.00 32.13 A C 44.123 44.524 31.194 1.00 29.05 A C 42.777 43.949 33.230 1.00 34.11 A C 39.911 42.132 30.271 1.00 28.16 A C 39.668 40.980 29.914 1.00 28.60 A O
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	176 N TYR 177 CA TYR 178 CB TYR 179 CG TYR 180 CD1 TYR 181 CE1 TYR 182 CD2 TYR	58 58 58 58 58 58 58	39. 394 43. 196 29. 676 1. 00 26. 69 A N 38. 530 43. 050 28. 518 1. 00 25. 82 A C 37. 071 42. 890 28. 934 1. 00 25. 51 A C 36. 195 42. 420 27. 797 1. 00 26. 86 A C 36. 051 41. 062 27. 514 1. 00 26. 92 A C 35. 294 40. 631 26. 429 1. 00 26. 28 A C 35. 557 43. 333 26. 965 1. 00 25. 26 A C 34. 803 42. 911 25. 882 1. 00 26. 13 A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	183 CE2 TYR 184 CZ TYR 185 OH TYR 186 C TYR 187 O TYR 188 N SER 189 CA SER 190 CB SER	58 58 58 58 59 59	34. 675 41. 564 25. 619 1. 00 25. 74 A C 33. 928 41. 160 24. 541 1. 00 27. 32 A 0 38. 681 44. 288 27. 647 1. 00 24. 95 A C 37. 837 45. 176 27. 680 1. 00 24. 68 A 0 39. 763 44. 338 26. 876 1. 00 24. 05 A N 40. 037 45. 470 25. 997 1. 00 24. 31 A C 41. 547 45. 657 25. 817 1. 00 24. 38 A C
ATOM ATOM ATOM ATOM ATOM	191 OG SER 192 C SER 193 O SER 194 N LEU 195 CA LEU	59 59 59 60 60	42. 187 45. 931 27. 051 1. 00 28. 99 A O 39. 405 45. 294 24. 628 1. 00 23. 54 A C 39. 795 44. 420 23. 860 1. 00 24. 84 A O 38. 430 46. 135 24. 319 1. 00 23. 51 A N 37. 765 46. 073 23. 031 1. 00 22. 96 A C

			FIG. 4-5	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	196 CB LEU 197 CG LEU 198 CD1 LEU 199 CD2 LEU 200 C LEU 201 O LEU 202 N ARG 203 CA ARG 204 CB ARG 205 CG ARG 206 CD ARG 207 NE ARG 209 NH1 ARG 210 NH2 ARG 211 C ARG 212 O ARG 211 C ARG 212 O ARG 213 N TRP 214 CA TRP 215 CB TRP 216 CG TRP 217 CD2 TRP 218 CE2 TRP 219 CE3 TRP 219 CE3 TRP 219 CE3 TRP 220 CD1 TRP 221 NE1 TRP 222 CZ2 TRP 223 CZ3 TRP 224 CH2 TRP 225 C TRP 226 O TRP 227 N ILE 228 CA ILE 230 CG2 ILE 230 CG2 ILE 231 CG1 ILE 232 CD1 ILE 233 C ILE 233 C ILE 234 O ILE 235 N SER	60 60 60 60 60 61 61 61 61 61 61 61 61 62 62 62 62 62 62 62 62 62 63 63 63 63 63 63 63	36. 256 45. 910 23. 228 1. 00 21. 27 35. 528 46. 977 24. 048 1. 00 20. 80 35. 373 48. 227 23. 208 1. 00 19. 95 34. 159 46. 466 24. 488 1. 00 18. 91 38. 072 47. 356 22. 279 1. 00 23. 42 38. 507 48. 340 22. 869 1. 00 25. 94 38. 102 48. 522 20. 153 1. 00 27. 08 39. 364 48. 323 19. 299 1. 00 29. 17 40. 545 47. 713 20. 076 1. 00 34. 91 41. 790 48. 612 20. 088 1. 00 38. 62 42. 423 48. 715 18. 772 1. 00 41. 15 43. 337 47. 871 18. 299 1. 00 41. 78 43. 754 46. 848 19. 033 1. 00 40. 61 43. 821 48. 042 17. 076 1. 00 43. 39 36. 869 48. 724 19. 270 1. 00 25. 92 36. 616 47. 939 18. 358 1. 00 24. 63 34. 883 50. 050 18. 794 1. 00 23. 22 33. 472 50. 900 <	A C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM	236 CA SER 237 CB SER 238 OG SER 239 C SER 240 O SER 241 N ASP	64 64 64 64 65	31. 510 51. 470 14. 768 1. 00 28. 43 30. 764 50. 603 13. 754 1. 00 27. 24 30. 181 49. 481 14. 392 1. 00 28. 00 30. 597 51. 727 15. 964 1. 00 29. 08 31. 008 51. 606 17. 119 1. 00 26. 71 29. 348 52. 067 15. 678 1. 00 31. 29	A C A C A O A C A O A N
ATOM ATOM ATOM	242 CA ASP 243 CB ASP 244 CG ASP	65 65 65	28. 382 52. 336 16. 732 1. 00 34. 90 27. 384 53. 397 16. 269 1. 00 37. 81 26. 515 53. 905 17. 395 1. 00 41. 52	A C A C A C

				FIG. 4-6		(Co	ontinued)
	•			FIG. 4-6		,	
ATOM	245	OD1 ASP	65	27.070 54.235 18.46			
ATOM	246	OD2 ASP	65	25. 281 53. 986 17. 21			
ATOM	247	C ASP	65	27.640 51.064 17.12			
ATOM	248	0 ASP	65	26.753 51.091 17.98			
ATOM	249	N HIS	66	28. 023 49. 946 16. 55 27. 369 48. 679 16. 80	07 1.00 35.30 A	_	
ATOM	250	CA HIS	66 66	_ · ·			
ATOM	251	CB HIS	66 66	26. 555 48. 229 15. 55 25. 648 49. 288 15. 0			, 1
MOTA	252	CG HIS	66	24. 298 49. 393 15. 0			,
ATOM ATOM	$\begin{array}{c} 253 \\ 254 \end{array}$	ND1 HIS	66	26. 121 50. 438 14. 4			
ATOM	25 4 255	CE1 HIS	66	25. 101 51. 206 14. 1			
ATOM	256	NE2 HIS	66	23. 984 50. 595 14. 4			
ATOM	257	C HIS	66	28. 314 47. 555 17. 2	23 1.00 33.78 A		
ATOM	258	0 HIS	66	27. 966 46. 736 18. 0			
ATOM	259	N GLU	67	29. 502 47. 501 16. 6			
ATOM	260	CA GLU	67	30. 432 46. 434 16. 9			
ATOM	261	CB GLU	67	30. 557 45. 463 15. 8			
ATOM	262	CG GLU	67	30. 356 46. 103 14. 4			
ATOM	263	CD GLU	67	30. 357 45. 092 13. 3		_	
ATOM	264	OE1 GLU	67	29.607 44.090 13.3 31.104 45.306 12.3			Ď
ATOM	265	OE2 GLU	67				
ATOM	266	C GLU	67 67	31. 818 46. 866 17. 4 32. 240 48. 003 17. 2			ő
ATOM	267 268	O GLU N TYR	68	32. 513 45. 940 18. 0			Ň
ATOM ATOM	269	CA TYR	68	33. 863 46. 190 18. 5			C
ATOM	270	CR TYR	68	33. 866 46. 447 20. 0			C
ATOM	271	CG TYR	68	33. 307 45. 324 20. 9		A (C
ATOM	272	CD1 TYR	68	32.000 45.376 21.4		A (C
ATOM	273	CE1 TYR	68	31.497 44.372 22.2			C
ATOM	274	CD2 TYR	68	34. 102 44. 232 21. 2			C
ATOM	275	CE2 TYR	68	33.610 43.225 22.1	110 1.00 22.67		C
ATOM	276	CZ TYR	68	32. 304 43. 305 22. 5			C .
ATOM	277	OH TYR	68	31.810 42.321 23.4			0 C
ATOM	278	C TYR	68	34.747 44.987 18.2			0
ATOM	279	0 TYR	68	34. 244 43. 885 18. 0 36. 058 45. 202 18. 2			N N
MOTA	280	N LEU CA LEU	69 69	36. 986 44. 115 17. 9		A .	C
ATOM	281 282	CA LEU CB LEU	69	38. 154 44. 602 17. 1			č
ATOM ATOM	283	CG LEU	69	37. 761 45. 065 15. 7		Ä	Č ·
ATOM	284	CD1 LEU	69	38. 978 45. 629 14. 9			C
ATOM	285	CD2 LEU	69	37. 164 43. 891 14. 9			C
ATOM	286	C LEU	69	37. 492 43. 588 19. 2	292 1.00 34.73		C
ATOM	287		69	37. 474 44. 305 20. 2			0
ATOM	288	N TYR	70	37. 927 42. 334 19. 3			N
ATOM	289	CA TYR	70	38. 423 41. 726 20.	•		C
ATOM	290		70	37. 251 41. 359 21. 4			C
ATOM	291	CG TYR	70	37. 689 40. 866 22. 7			C
ATOM	292		70	38.400 41.697 23.6 38.837 41.253 24.8			C C
ATOM	293	CE1 TYR	70	38. 837 41. 253 24. 8	000 1.00 TT.UJ	11	v

				FIG. 4-7		(Continued)
ATOM	294	CD2 TYR	70	37. 421 39. 563 23. 213 1.	. 00 43. 93 A	С
ATOM	295	CE2 TYR	70	37. 853 39. 104 24. 452 1.	.00 44.83 A	C
ATOM	296	CZ TYR	70	38. 563 39. 959 25. 286 1.	.00 45.17 A	C
ATOM	297	OH TYR	70		. 00 47. 21 A	0
ATOM	298	C TYR	70	• • • • • • • • • • • • • • • • • • • •	.00 45.46 A	C
ATOM	299	O TYR	70		. 00 46. 31 A	0
ATOM	300	N LYS	71		.00 49.93 A	N
ATOM	301	CA LYS	71	*****	. 00 54. 71 A	C
ATOM	302	CB LYS	71		. 00 54.14 A	C
ATOM	303	CG LYS	71		. 00 56.37 A	C
ATOM	304	CD LYS	71		. 00 58. 61 A	C
ATOM	305	CE LYS	71		. 00 58. 78 A . 00 60. 82 A	N N
ATOM	306	NZ LYS	71	==: : : : :	. 00 60. 82 A . 00 57. 38 A	C
ATOM	307	C LYS	71		1.00 57.38 A	ŏ
ATOM	308	O LYS	71	=-:-:	1.00 56.30 A	Ň
ATOM	309	N GLN	72		1.00 63.23 A	Ċ
ATOM	310	CA GLN CB GLN	$\begin{array}{c} 72 \\ 72 \end{array}$		1.00 64.07 A	Č
ATOM	311 312	CG GLN	72		i. 00 65. 84 A	Č
ATOM ATOM	313	CD GLN	72	37. 270 34. 240 23. 375 1	1.00 66.33 A	
ATOM	314	OE1 GLN	72		1.00 67.19 A	
ATOM	315	NE2 GLN	72		I. 00 66. 80 A	
ATOM	316	C GLN	72		I. 00 65. 34 A	
ATOM	317	O GLN	72		1.00 67.00 A	
ATOM	318	N GLU	73	41.736 34.442 21.597 1	1.00 66.09 A	
ATOM	319	CA GLU	73		1.00 67.12 A	C
ATOM	320	CB GLU	73	= = = :	1.00 68.53 A	
ATOM	321	CG GLU	73		1.00 71.35 A	
ATOM	322	CD GLU	73		1.00 72.71 A	
ATOM	323	OE1 GLU	73		1.00 73.51 A	
ATOM	324	OE2 GLU	73		1.00 74.16 A	
ATOM	325	C GLU	73		1.00 66.83 A	
ATOM	326	O GLU	73		1.00 67.65 A	
ATOM	327	N ASN	74		1. 00 65. 38 A 1. 00 63. 38 A	
ATOM	328	CA ASN	74	••••	1.00 63.38	_
ATOM	329	CB ASN	74		4 00 00 10 4	
ATOM	330	CG ASN	74	+ · · · · · · · · · · · · · · · · · · ·	1.00 66.10 A 1.00 65.51 A	
ATOM	331	OD1 ASN	74		1.00 66.62 A	
ATOM	332	ND2 ASN C ASN	74 74		1.00 61.55 A	
ATOM	333		74		1.00 62.15 A	
ATOM	334 335	O ASN N ASN	75		1.00 58.67 A	
ATOM ATOM	336	CA ASN	75		1.00 55.82 A	
ATOM	337	CB ASN	75		1.00 57.81 A	_
ATOM	338	CG ASN	75		1.00 58.63 A	
ATOM	339	OD1 ASN	75	40.857 34.358 17.909	1.00 59.69 A	. 0
ATOM	340	ND2 ASN	75	41,500 32,580 16,697	1.00 58.92 A	
ATOM	341	C ASN	7Š	42.017 37.045 16.918	1.00 52.82 A	
ATOM	342		75	41.630 37.135 18.081	1.00 53.60 A	. 0

F I G. 4 - 8	
ATOM 344 CA ILE 76	

					FΙ	G. 4	- 9			(Continu	ued)
ATOM	202	CD (וו זי	82	22.602	44. 794	19.655	1.00 36.97	Α	С	
ATOM ATOM	392 393		GLU GLU	82 82	21.115	44. 827	19.968	1.00 40.49	Α	C	
ATOM	394		GLU	82	20. 313	45.538	18.894	1.00 44.05	Α	C	
ATOM	395	0E1 (82	20. 343	45.087	17.726	1.00 45.13	Α	0	
ATOM	396	0E2 (82	19.652	46.551	19.220	1.00 45.61	Α	0	
ATOM	397		GLU	82	23.042	42.853	21.153	1.00 33.95	Α	C	
ATOM	398		GLU	82	22.055	42.662	21.864	1.00 32.29	A	0	
ATOM	399		TYR	83	23.777	41.857	20.666	1.00 33.23	A	N	
ATOM	400		TYR	83	23.423	40.468	20.947	1.00 33.39	A	C	
ATOM	401		TYR	83	22.846	39.810	19.686	1.00 34.54	A	C	
ATOM	402	CG	TYR	83	21.690	40.594	19. 109	1.00 34.80	A	C	
ATOM	403		TYR	83	20. 558	40.859	19.878	1.00 35.22	A	C	
ATOM	404		TYR	83	19. 527	41.657	19.396	1.00 36.27	A	C	
ATOM	405	CD2		83	21.759	41.139	17.828	1.00 35.71	A A	C C	
ATOM	406	CE2		83	20. 731	41.940	17. 331	1.00 37.42 1.00 37.70	A	C	
ATOM	407		TYR	83	19.619	42.200	18.125	1.00 37.70	A	0	
ATOM	408		TYR	83	18. 624	43.044 39.644	17.675 21.494	1.00 31.09	A	Č	
ATOM	409		TYR	83	24. 582	38.511	21. 434	1.00 32.91	A	ŏ	
ATOM	410		TYR	83	24. 396 25. 777	40. 217	21. 476	1.00 33.53	A	N	
ATOM	411		GLY	84	26. 933	39.513	21.995	1.00 33.40	A	Ċ	•
ATOM	412		GLY GLY	84 84	27. 454	38. 395	21.114	1.00 33.92	Ä	Č	
ATOM	413 414		GLY	84	28. 329	37.639	21.530	1.00 33.21	Ä	Ö	
ATOM ATOM	414		ASN	85	26. 918	38. 269	19.904	1.00 35.26	A	N	
ATOM	416		ASN	85	27. 388	37. 233	18. 993	1.00 37.43	Α	C	
ATOM	417		ASN	85	26. 258	36.780	18.072	1.00 38.34	Α	C	
ATOM	418		ASN	85	25. 764	37.878	17.166	1.00 40.02	Α	C	
ATOM	419	0D1		85	25.694	39.040	17.561	1.00 39.96	Α	0	
ATOM	420	ND2	ASN	85	25. 394	37.496	15.950	1.00 41.91	Α	N	
ATOM	421	C	ASN	85	28.556	37.794	18. 188	1.00 38.80	A	Ç	
ATOM	422	Ŏ	ASN	85	28.687	39.011	18.035	1.00 40.05	A	0	
ATOM	423	N	SER	86	29.410	36.920	17.670	1.00 39.14	A	N	
ATOM	424	CA	SER	86	30. 565	37.393	16.926	1.00 39.30	A	C	
ATOM	425	CB	SER	86 .	31. 723	37. 587	17.895	1.00 38.90	A	C	
ATOM	426	0G	SER	86	32. 041	36.356	18. 515	1.00 35.77	A	0	
ATOM	427	C	SER	86	31.023	36. 482	15.798	1.00 39.94	A	C	
MOTA	428		SER	86	30. 287	35. 622	15. 323	1.00 41.15	A	0 N	
ATOM	429	N	SER	87	32. 264	36. 701	15. 382	1.00 40.59	A	N C	
ATOM	430	CA	SER	87	32. 916	35. 929	14. 333	1.00 40.98	A A	Č	
ATOM	431	CB	SER	87	32. 152	36.053	13.010	1.00 39.16 1.00 39.90	A	Õ	
ATOM	432		SER	87	31. 727	37. 376	12. 789 14. 194		A	Č	
ATOM	433		SER	87	34. 353	36. 433	14. 194	1.00 41.10	A	ŏ	
ATOM	434		SER	87	34. 691	37. 517 35. 646	13.548		A	N	
ATOM	435		VAL	88	35. 206 36. 596	36. 043	13. 402		A	Č	
ATOM	436		VAL	88	37. 502	34. 836	13. 114		Ä	č	
ATOM	437		VAL	88 88	38. 949	35. 295	13.013		A	č	
ATOM	438		VAL	88	37. 361	33. 808	14. 222		A	Č	
ATOM	439		VAL	88	36. 827	37. 096		1.00 41.63	A	Č	
ATOM	440	U	VAL	00	00.041	01.000	12.001	<u> </u>			

	•			(Continued)
			FIG. 4-10	(00220
				•
ATOM	441 0 VAL	88	36. 548 36. 885 11. 154 1. 00 41. 38 A	
ATOM	442 N PHE	89	37. 343 38. 238 12. 767 1. 00 42. 23 A	_
ATOM	443 CA PHE	89	37. 641 39. 347 11. 880 1. 00 42. 51 A	
ATOM	444 CB PHE	89	01.100 10.001 12.00	
ATOM	445 CG PHE	89	41.000	
ATOM	446 CD1 PHE	89	400 40 00	
ATOM	447 CD2 PHE	89	100 00 00	
ATOM	448 CE1 PHE	89	4 00 00 07	
ATOM	449 CE2 PHE	89	37. 154 43. 911 10. 894 1. 00 39. 87 A 38. 381 44. 135 10. 295 1. 00 39. 50 A	
ATOM	450 CZ PHE	89	38. 956 39. 021 11. 186 1. 00 43. 57	_
ATOM	451 C PHE	89 89	39. 156 39. 335 10. 019 1. 00 43. 51 A	2
ATOM	452 O PHE 453 N LEU	90	39. 851 38. 376 11. 921 1. 00 45. 92	
ATOM	453 N LEU 454 CA LEU	90	41. 143 38. 001 11. 380 1. 00 48. 60	A C
ATOM	455 CB LEU	90	42. 071 39. 213 11. 366 1. 00 48. 66	
ATOM ATOM	456 CG LEU	90	43. 033 39. 305 10. 184 1. 00 49. 47	
ATOM	457 CD1 LEU	90	42. 236 39. 408 8. 889 1. 00 50. 17	A C
ATOM	458 CD2 LEU	90	43. 933 40. 515 10. 346 1. 00 49. 94 <i>I</i>	A C
ATOM	459 C LEU	90	41.718 36.907 12.267 1.00 50.84	A C
ATOM	460 O LEU	90	42.000 01.100 10.11	A 0
ATOM	461 N GLU	91	11.010	A N
ATOM	462 CA GLU	91	12.000	A C A C
ATOM	463 CB GLU	91	11.01, 00.010	
ATOM	464 CG GLU	91	12.010	A C A C
ATOM	465 CD GLU	91		A O
ATOM	466 OE1 GLU	91		A 0
ATOM	467 OE2 GLU	91		A Č
ATOM	468 C GLU	91	43. 855 34. 521 12. 588 1. 00 56. 96 44. 572 34. 841 11. 641 1. 00 56. 93	A Ö
ATOM	469 O GLU	91 92		A N
ATOM	470 N ASN 471 CA ASN	92		A C
ATOM	471 CA ASN 472 CB ASN	92	10.100 01.020	A C
ATOM ATOM	473 CG ASN	92		A C
ATOM	474 OD1 ASN	92		A 0
ATOM	475 ND2 ASN	92	44.420 31.894 16.691 1.00 61.11	A N
ATOM	476 C ASN	92	46.622 33.271 13.111 1.00 59.58	A C
ATOM	477 O ASN	92	41.000	A 0
ATOM	478 N SER	93	10.000	A N
ATOM	479 CA SER	93	10.000	A C
ATOM	480 CB SER	93	10.010	A C
ATOM	481 OG SER	93	46.714 30.198 9.507 1.00 64.10	A 0
ATOM	482 C SER	93	47. 296 33. 030 9. 853 1. 00 62. 23	A C A 0
ATOM	483 O SER	93	48. 314 32. 765 9. 213 1. 00 62. 82	
ATOM	484 N THR	94	46. 552 34. 103 9. 618 1. 00 62. 37 46. 852 35. 036 8. 541 1. 00 62. 69	A N A C
ATOM	485 CA THR	94	10.00	A C
ATOM	486 CB THR	94	100 00 50	A O
ATOM	487 OG1 THR	94	10.10	A Č
ATOM	488 CG2 THR	94 04	46.003 36.821 10.080 1.00 64.14 48.306 35.464 8.377 1.00 62.28	A C
ATOM	489 C THR	94	40.000 00.404 0.011 1.00 05.00	

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										(Continued)
					FΙ	G. 4	- 11			(00=01====
ATOM ATOM	491		THR PHE	94 95	48. 882 48. 908	35, 295 36, 013	7. 303 9. 426	1.00 61.92 1.00 62.57	A A	0 N
ATOM ATOM	493	CB	PHE PHE	95 95	50. 290 50. 414	36. 473 37. 889	9. 322 9. 897	1.00 63.04 1.00 61.98	A A	C C
ATOM ATOM		CG CD1	PHE PHE	95 95	49. 456 48. 248	38. 869 39. 155	9. 289 9. 911	1.00 61.01 1.00 60.97	A A	C C
ATOM	496	CD2	PHE	95	49.742	39.473	8.073	1.00 60.73	A	C C
ATOM ATOM		CE1 CE2		95 95	47. 337 48. 838	40. 026 40. 343	9. 330 7. 483	1.00 60.46 1.00 60.09	A A	С
ATOM	499	CZ	PHE	95	47.633	40.621	8.113	1.00 61.07	A	С
ATOM ATOM		C 0	PHE PHE	95 95	51.346 52.178	35. 571 36. 035	9.956 10.736	1.00 63.20 1.00 63.66	A A	C 0
ATOM	502	N	ASP	96	51.323	34. 288	9.611	1.00 63.37	A	N
ATOM ATOM		CA CB	ASP ASP	96 96	52. 298 51. 771	33. 347 31. 913	10.149 10.044	1.00 64.05 1.00 65.11	A A	C C
ATOM	50 5	CG	ASP	96	50.747	31.589	11.115	1.00 65.73	A	C 0
ATOM ATOM		0D1 0D2		96 96	49. 758 50. 929	32. 342 30. 580	11. 240 11. 829	1.00 66.41 1.00 65.32	A A	0
ATOM	508	C	ASP	96	53.621	33.470	9.399 10.001	1.00 63.82 1.00 64.05	A A	C 0
ATOM ATOM		O N	ASP GLU	96 97	54. 696 53. 540	33. 433 33. 619	8.083	1.00 62.95	A	N
ATOM	511	CA CB	GLU GLU	97	54. 740 54. 596	33. 754 32. 964	7. 271 5. 965	1.00 62.73 1.00 65.91	A A	C C
ATOM ATOM		CG	GLU	.97 97	54. 954	31.478	6.064	1.00 68.84	A	С
ATOM		CD 0E1	GLU	97 97	53. 945 54. 160	30. 657 29. 432	6.850 6.988	1.00 70.64 1.00 71.38	A A	C 0
ATOM ATOM			GLU	97	52. 939	31. 228	7. 325	1.00 71.80	A	0
ATOM		C	GLU GLU	97 97	55. 039 55. 462	35. 220 35. 557	6.963 5.857	1.00 60.82 1.00 60.31	A A	C 0
ATOM ATOM		0 N	PHE	98	54. 818	36.084	7.952	1.00 58.68	A	N
ATOM ATOM	520 521	CA CB	PHE PHE	98 98	55. 067 54. 200	37. 513 38. 319	7. 797 8. 765	1.00 55.93 1.00 55.47	A A	C
ATOM	522	CG	PHE	98	54. 272	39. 801	8.542	1.00 54.84	Α	č
ATOM ATOM	523 524		PHE PHE	98 98	53. 712 54. 931	40. 372 40. 624	7. 404 9. 450	1. 00 53. 07 1. 00 53. 89	A A	C C C C
ATOM	525	CE1	PHE	98	53.808	41.743	7.173	1.00 53.28	Α	С
ATOM ATOM		CE2 CZ	PHE PHE	98 98	55. 032 54. 470	41. 997 42. 556	9. 226 8. 087	1. 00 53. 18 1. 00 52. 22	A A	C C
ATOM	528	C	PHE	98	56. 536	37.820	8.060	1.00 54.61	Α	C
ATOM ATOM		0 N	PHE GLY	98 99	57. 041 57. 215	38. 878 36. 885	7. 686 8. 713	1.00 53.80 1.00 53.53	A A	0 N
ATOM	531	CA	GLY	99	58.624	37.061	9.004	1.00 52.08	Α	N C C
ATOM ATOM	532 533	C 0	GLY GLY	99 99	58. 908 60. 037	38. 188 38. 673	9. 972 10. 051	1.00 51.18 1.00 51.30	A A	C 0
ATOM	534	N	HIS	100	57.884	38.607	10.706	1.00 50.21	Α	N
ATOM ATOM	535 536	CA CB	HIS HIS	100 100	58. 026 57. 810	39. 681 41. 049	11.686 11.028	1.00 49.15 1.00 48.84	A A	C C
ATOM	537	CG	HIS	100	58. 850	41.410	10.014	1.00 49.22	Α	С
ATOM	538	CD2	HIS	100	58. 759	41.613	8. 679	1.00 49.42	A	С

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ATOM

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(Continued) FIG. 4-12 ξ, 41.627 10.346 1.00 49.70 A N ND1 HIS 100 60.170 ATOM 539 41.951 9.259 1.00 49.10 A C CE1 HIS 60.848 **ATOM** 540 100 60.015 41.949 8.234 1.00 50.14 A N 100 541 NE2 HIS **ATOM** C 57.011 39.511 12.810 1.00 48.06 A HIS 100 542 C **ATOM** 55.920 38.977 12.602 1.00 47.18 A 0 HIS 0 100 **ATOM** 543 57.377 39.958 14.005 1.00 46.66 A N SER 101 **ATOM** 544 N C 39.878 15.136 1.00 45.88 A 56.467 SER 101 **ATOM** 545 CA C 39.802 16.446 1.00 47.41 A 57.247 CB SER 101 **ATOM** 546 58.118 38.685 16.447 1.00 51.04 A 0 ATOM 547 0G SER 101 41.142 15.112 1.00 44.53 A C 55.617 101 548 C SER **ATOM** 0 56.133 42.248 15.282 1.00 44.41 A 0 SER 101 549 ATOM 40.976 14.877 1.00 41.90 N 54.319 A ILE 102 N **ATOM** 550 53.409 42.109 14.833 1.00 38.95 C A CA ILE 102 ATOM 551 C 41.732 14.117 1.00 38.54 52.106 A 102 **ATOM** 552 CB ILE Ċ 1.00 38.18 51.153 42.926 14.103 A CG2 ILE **ATOM** 553 102 41.288 12.686 1.00 37.65 A 52.424 **ATOM** 554 CG1 ILE 102 C 40.733 11.937 1.00 37.11 A CD1 ILE 102 51.243 **ATOM** 555 C 1.00 38.00 42.597 16.244 556 ILE 102 53.104 A **ATOM** C 0 41.919 17.024 1.00 38.06 557 0 ILE 102 52.441 A **ATOM** 53.601 43.787 16.556 1.00 37.54 Α N ASN 103 **ATOM** 558 N 53.429 44.399 C 17.867 1.00 36.65 A ASN 103 **ATOM** 559 CA 1.00 37.69 C 54.437 45.530 18.039 A ASN 103 560 CB **ATOM** 54.219 46.308 1.00 39.56 C 19.315 A ASN 561 CG 103 **ATOM** 54.655 45.891 20.388 1.00 43.00 0 A OD1 ASN **ATOM** 562 103 1.00 38.34 N 53.528 47.439 19.211 A ND2 ASN 103 **ATOM** 563 C 52.031 44.953 18.116 1.00 35.79 A **ASN** 564 C 103 **ATOM** 51.532 44.910 19.237 1.00 35.79 Α 0 ASN 565 103 **ATOM** 0 51.405 45.490 17.078 N 1.00 34.43 A 566 N ASP 104 **ATOM** C 50.079 46.067 17.236 1.00 33.27 A CA ASP 104 ATOM 567 1.00 34.38 C 50.200 47.388 17.998 ASP A **ATOM** CB 104 568 C 48.896 47.823 18.618 1.00 34.79 A ASP 569 CG 104 **ATOM** 0 48.699 19.509 1.00 33.92 A ATOM OD1 ASP 48.916 104 570 18.207 47.289 1.00 36.80 0 OD2 ASP 47.852 A 571 104 **ATOM** 1.00 32.32 49.436 46.281 15.865 C **ASP** A 572 C 104 **ATOM** 50.124 46.326 14.850 1.00 32.03 0 A ASP 104 **ATOM** 573 0 1.00 31.15 15.834 48.118 46.405 N 574 **TYR** 105 Α **ATOM** N 47.421 46.580 14.570 1.00 32.24 C 105 A **ATOM** 575 CA TYR 46.672 45.296 14.223 1.00 34.70 A C **ATOM** 576 CB TYR 105 C 45.443 45.088 15.072 1.00 37.73 Α **TYR** 105 ATOM 577 CG 44.220 45.636 14.698 1.00 37.51 A C 578 CD1 TYR 105 **ATOM** 43.098 45.510 15.506 1.00 40.43 A C ATOM 579 CE1 TYR 105 45.514 44.395 16.284 C 1.00 39.06 **ATOM** A 580 CD2 TYR 105 44.263 17.103 C 1.00 40.75 44.393 A **ATOM** 581 CE2 TYR 105 C 44.829 16.705 1.00 41.19 43.191 Α 582 CZTYR 105 ATOM 44.755 17.519 1.00 44.27 A 0 42.088 **ATOM** 583 OH TYR 105 C 1.00 31.43 47.743 14.638 A **ATOM** 584 C TYR 105 46.441 1.00 30.78 0 48.249 15.715 A 585 TYR 105 46.133 ATOM 0 13.479 1.00 30.16 N 48.152 586 106 45.940 Α ATOM N SER

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A

			FIG. 4-13	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	588 CB SER 589 OG SER 590 C SER 591 O SER 591 O SER 592 N ILE 593 CA ILE 594 CB ILE 595 CG2 ILE 596 CG1 ILE 597 CD1 ILE 598 C ILE 599 O ILE 599 O ILE 600 N SER 601 CA SER 602 CB SER 603 OG SER 604 C SER 605 O SER 606 N PRO 607 CD PRO 608 CA PRO 607 CD PRO 608 CA PRO 610 CG PRO 610 CG PRO 611 C PRO 612 O PRO 610 CG PRO 611 C PRO 612 O PRO 611 C PRO 612 O PRO 613 N ASP 614 CA ASP 615 CB ASP 616 CG ASP 617 OD1 ASP 618 OD2 ASP 619 C ASP 619 C ASP 610 CG ASP 617 OD1 ASP 618 OD2 ASP 619 C ASP 610 CG ASP 610 CG ASP 611 C PRO 612 O PRO 613 N ASP 614 CA ASP 615 CB ASP 616 CG ASP 617 OD1 ASP 618 OD2 ASP 619 C ASP 619 C ASP 620 O ASP 621 N GLN 622 CA GLN 623 C GLN 624 O GLN 625 N GLN 626 CA GLN 627 CB GLN 628 CG GLN 629 CD GLN 630 OE1 GLN 631 NE2 GLN 632 C GLN 633 O GLN 634 N PHE 635 CA PHE	111 111 112 112 112 112 112 112 112 112	45. 762 50. 588 13. 457 1. 00 29. 8 44. 924 51. 668 13. 090 1. 00 32. 3 44. 146 49. 187 12. 157 1. 00 27. 6 44. 657 49. 085 11. 051 1. 00 28. 5 42. 835 49. 240 12. 331 1. 00 28. 6 41. 922 49. 171 11. 198 1. 00 27. 7 40. 648 48. 352 11. 544 1. 00 25. 8 39. 557 48. 620 10. 522 1. 00 26. 3 41. 980 46. 457 12. 568 1. 00 23. 7 41. 980 46. 457 12. 568 1. 00 23. 7 41. 138 51. 420 11. 557 1. 00 26. 8 41. 178 51. 420 11. 557 1. 00 26. 8 41. 133 52. 035 8. 862 1. 00 26. 8 41. 331 52. 033 7. 346 1. 00 26. 8 41. 331 52. 033 7. 346 1. 00 26. 8 41. 331 52. 033 7. 346 1. 00 26. 8 40. 458 51. 119 6. 700 1. 00 23. 6 39. 241 53. 506 9. 393 1. 00 27. 3 38. 857 51. 310 9. 206 1. 00 26. 8 40. 025 54. 751 9. 302 1. 00 29. 37. 839 53. 794 9. 693 1. 00 29. 37. 839 53. 794 9. 693 1. 00 29. 37. 839 53. 794 9. 693 1. 00 29. 37. 839 55. 775 9. 899 1. 00 30. 39. 080 55. 775 9. 899 1. 00 30. 39. 080 55. 775 9. 899 1. 00 28. 36. 842 52. 993 8. 852 1. 00 29. 37. 046 52. 935 7. 540 1. 00 29. 36. 120 52. 202 6. 676 1. 00 28. 36. 241 52. 673 5. 226 1. 00 27. 37. 613 52. 425 9. 391 1. 00 30. 37. 046 52. 935 7. 540 1. 00 29. 36. 120 52. 202 6. 676 1. 00 28. 36. 241 52. 673 5. 226 1. 00 27. 37. 613 52. 432 4. 648 1. 00 27. 38. 226 51. 397 4. 976 1. 00 29. 35. 635 49. 971 5. 953 1. 00 30. 37. 148 50. 196 7. 589 1. 00 28. 37. 349 48. 766 7. 702 1. 00 28. 37. 349 48. 766 7. 702 1. 00 28. 37. 349 48. 766 7. 702 1. 00 28. 37. 349 48. 766 7. 702 1. 00 28. 37. 349 48. 766 7. 702 1. 00 28. 37. 349 48. 766 7. 702 1. 00 28. 37. 349 48. 766 7. 702 1. 00 28. 37. 349 48. 766 7. 702 1. 00 28. 37. 349 48. 766 7. 702 1. 00 29. 37. 336 49. 442 2. 749 1. 00 31. 37. 148 50. 196 7. 589 1. 00 31. 37. 148 50. 196 7. 589 1. 00 31. 37. 148 50. 196 7. 589 1. 00 31. 37. 148 50. 196 7. 589 1. 00 31. 37. 148 50. 196 7. 589 1. 00 31. 37. 148 50. 196 7. 589 1. 00 31. 37. 148 50. 196 7. 589 1. 00 31. 37. 148 50. 196 7. 589 1. 00 31. 37. 148 50. 196 7. 589 1. 00 31. 37. 148 50. 196 7. 589 1. 00 31. 37. 148 50. 196 7. 589 1. 00 31. 37. 148 50. 196 7. 589 1. 00 31. 37. 148 50. 196	12

				(Continued)
			FIG. 4-15	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	686 CZ TYR 687 OH TYR 688 C TYR 689 O TYR 690 N ASN 691 CA ASN 691 CA ASN 692 CB ASN 693 CG ASN 694 OD1 ASN 695 ND2 ASN 696 C ASN 697 O ASN 699 CA TYR 700 CB TYR 700 CB TYR 701 CG TYR 702 CD1 TYR 702 CD1 TYR 703 CE1 TYR 704 CD2 TYR 705 CE2 TYR 706 CZ TYR 707 OH TYR 708 C TYR 707 OH TYR 708 C TYR 708 C TYR 709 O TYR 710 N VAR 711 CA VAR 712 CB VAR 713 CG1 VAR 714 CG2 VAR 715 C VAR 716 O VAR 717 N LY 718 CA LY 719 CB LY	R 118 R 118 R 118 R 119 R 119 N 119 N 119 N 119 N 119 R 120 L 121 S 122 S 122	FIG. 4 - 15 57. 459	(Continued) A C A O A C A O A N A C A C A C A C A C A C A C A C A C A C
ATOM ATOM ATOM	720 CG LY 721 CD LY 722 CE LY	S 122 S 122 S 122	59. 793 52. 954 24. 819 1. 00 21. 38 59. 573 52. 354 26. 191 1. 00 20. 47 59. 078 53. 406 27. 174 1. 00 19. 23	A C A C A C A N
ATOM ATOM ATOM ATOM	723 NZ LY 724 C LY 725 O LY 726 N GL	'S 122 'S 122 .N 123	61. 460 53. 635 22. 528 1. 00 27. 64 62. 658 53. 464 22. 315 1. 00 28. 10 60. 947 54. 813 22. 860 1. 00 27. 23	A C A O A N A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	727 CA GL 728 CB GL 729 CG GL 730 CD GL 731 OE1 GL 732 NE2 GL 733 C GL	.N 123 .N 123 .N 123 .N 123 .N 123 .N 123	61. 607 57. 034 21. 974 1. 00 28. 29 62. 537 58. 227 22. 164 1. 00 28. 94 62. 339 59. 308 21. 131 1. 00 29. 91 61. 218 59. 744 20. 889 1. 00 32. 37 63. 431 59. 761 20. 524 1. 00 30. 94 61. 385 56. 545 24. 428 1. 00 26. 89	A C A C A C A O A N A C
ATOM	734 O GL	N 123	61.837 56.036 25.453 1.00 27.03	A 0

(Continued)

ATOM 735 N TRP 124 60.081 58.149 25.713 1.00 24.21 A C ATOM 737 CB TRP 124 60.081 58.149 25.713 1.00 24.21 A C ATOM 738 CG TRP 124 61.052 60.357 24.934 1.00 19.79 A C ATOM 738 CG TRP 124 61.052 60.357 24.934 1.00 19.79 A C ATOM 739 CDZ TRP 124 62.444 60.061 25.127 1.00 19.03 A C ATOM 740 CE2 TRP 124 63.175 60.913 24.270 1.00 19.03 A C ATOM 740 CE2 TRP 124 63.175 60.913 24.270 1.00 19.03 A C ATOM 741 CE3 TRP 124 63.175 60.913 24.270 1.00 19.13 A C ATOM 742 CDJ TRP 124 62.270 61.509 23.597 1.00 18.84 A C ATOM 744 CZZ TRP 124 64.531 69.99 61.350 24.006 1.00 18.84 A C ATOM 744 CZZ TRP 124 64.531 69.192 25.800 1.00 17.77 A C ATOM 745 CZ3 TRP 124 64.533 59.129 25.800 1.00 17.77 A C ATOM 746 CH2 TRP 124 65.229 59.886 24.996 1.00 17.77 A C ATOM 746 CH2 TRP 124 65.229 59.886 24.996 1.00 17.07 A C ATOM 746 CH2 TRP 124 65.229 59.886 24.996 1.00 17.07 A C ATOM 746 CH2 TRP 124 65.229 59.886 24.996 1.00 17.07 A C ATOM 746 CH2 TRP 124 65.229 59.886 24.996 1.00 17.07 A C ATOM 747 C TRP 124 58.787 57.494 26.209 1.00 24.57 A C ATOM 748 0 TRP 124 58.787 57.494 26.209 1.00 24.57 A C ATOM 749 N ARC 125 56.189 58.183 58.212 27.013 1.00 24.35 A N C ATOM 750 CA ARG 125 56.189 58.621 28.609 1.00 23.81 A C ATOM 750 CA ARG 125 56.189 58.621 28.609 1.00 23.81 A C ATOM 750 CA ARG 125 56.935 88.652 128.609 1.00 23.81 A C ATOM 750 CA ARG 125 56.935 88.652 128.609 1.00 23.81 A C ATOM 750 CA ARG 125 56.935 88.657 29.308 1.00 23.85 A C ATOM 756 NH1 ARG 125 56.051 59.573 31.289 1.00 23.85 A C ATOM 756 NH1 ARG 125 56.051 59.575 31.289 1.00 23.85 A C ATOM 756 NH1 ARG 125 56.051 59.575 31.289 1.00 23.85 A C ATOM 757 NH2 ARG 125 56.935 58.865 79.31 289 1.00 23.85 A C ATOM 768 C HIS 126 55.293 58.867 23.775 1.00 23.399 A N ATOM 767 NE2 HIS 126 55.293 58.867 23.775 1.00 23.399 A N ATOM 767 NE2 HIS 126 55.293 58.867 23.775 1.00 23.399 A N ATOM 767 NE2 HIS 126 55.295 59.930 24.433 1.00 22.42 A N ATOM 769 O HIS 126 55.295 59.930 24.433 1.00 22.44 A C ATOM 769 O HIS 126 55.295 59.930 24.433 1.00 22.44 A C ATOM 769 O HIS 126 55.295 59.930 24.433 1.00 22.44						मा	G 4 -	1 6			(Cont
ATOM 736 CA TRP 124 60.081 58.149 25.713 1.00 24.21 A C ATOM 737 CB TRP 124 61.052 60.081 58.149 25.713 1.00 23.25 A C ATOM 738 CD TRP 124 61.052 60.587 24.934 1.00 19.79 A C C ATOM 739 CD2 TRP 124 61.052 60.587 24.934 1.00 19.79 A C C ATOM 740 CE2 TRP 124 63.1475 60.913 24.270 1.00 19.03 A C C ATOM 741 CE3 TRP 124 63.1475 60.913 24.270 1.00 19.03 A C C ATOM 741 CE3 TRP 124 63.145 59.157 25.936 1.00 15.51 A C C ATOM 742 CD1 TRP 124 60.999 61.350 24.006 1.00 18.84 A C C ATOM 742 CD1 TRP 124 62.270 61.690 23.597 1.00 18.74 A N C ATOM 744 CZ2 TRP 124 64.571 60.885 24.196 1.00 17.77 A C C ATOM 745 CZ2 TRP 124 65.229 59.866 24.996 1.00 17.77 A C C ATOM 746 CH2 TRP 124 65.229 59.866 24.996 1.00 17.77 A C C ATOM 747 C TRP 124 58.787 57.494 26.209 1.00 24.57 A C ATOM 748 O TRP 124 58.490 56.350 25.861 1.00 25.71 A O ATOM 748 O TRP 124 58.490 56.350 25.861 1.00 24.57 A C ATOM 749 N ARG 125 56.193 58.621 28.609 1.00 24.36 A N ATOM 750 CA ARG 125 56.193 58.621 28.609 1.00 23.36 A C C ATOM 751 CB ARG 125 56.193 58.621 28.609 1.00 23.36 A C C ATOM 752 CG ARG 125 56.193 58.621 28.609 1.00 23.36 A C C ATOM 753 CD ARG 125 54.953 58.065 29.308 1.00 23.35 A C C ATOM 755 NIH ARG 125 56.051 59.357 33.347 1.00 24.36 A C ATOM 755 NIH ARG 125 56.051 59.357 33.347 1.00 24.40 A C ATOM 756 NIH ARG 125 56.051 59.357 33.347 1.00 24.40 A C ATOM 757 NIE ARG 125 56.051 59.357 33.347 1.00 24.40 A C ATOM 757 NIE ARG 125 54.953 58.063 25.861 1.00 25.04 A C ATOM 760 N HIS 126 55.065 59.357 33.347 1.00 24.40 A C ATOM 760 N HIS 126 55.065 59.357 33.347 1.00 24.40 A C ATOM 760 N HIS 126 55.065 59.357 33.347 1.00 24.40 A C ATOM 760 N HIS 126 55.065 59.357 33.347 1.00 24.40 A C ATOM 760 N HIS 126 55.065 59.357 33.347 1.00 24.40 A C ATOM 760 N HIS 126 55.065 59.357 33.347 1.00 24.40 A C ATOM 760 N HIS 126 55.065 59.357 30.34 24.05 1.00 23.35 A C ATOM 760 N HIS 126 55.065 59.357 33.347 1.00 24.43 A N ATOM 760 N HIS 126 55.202 60.064 27.532 1.00 23.39 A N ATOM 760 N HIS 126 55.202 60.064 27.532 1.00 23.39 A N ATOM 760 N HIS 126 55.205 60.360 32.274 1.00											N
ATOM 737 CB TRP 124 59.886 59.665 25.572 1.00 23.25 A C ATOM 738 CC TRP 124 61.652 60.357 24.934 1.00 19.79 A C ATOM 739 CD2 TRP 124 63.175 60.913 24.270 1.00 19.03 A C C ATOM 740 CE2 TRP 124 63.175 60.913 24.270 1.00 19.03 A C C ATOM 740 CE2 TRP 124 63.175 60.913 24.270 1.00 19.13 A C C ATOM 741 CE3 TRP 124 63.143 59.157 25.936 1.00 15.51 A C ATOM 742 CD1 TRP 124 62.270 61.690 23.597 1.00 18.74 A N C ATOM 743 NE1 TRP 124 62.270 61.690 23.597 1.00 18.74 A N C ATOM 743 NE1 TRP 124 64.571 60.885 24.196 1.00 17.77 A C C ATOM 746 CH2 TRP 124 65.229 59.986 24.996 1.00 17.07 A C ATOM 746 CH2 TRP 124 65.229 59.986 24.996 1.00 17.07 A C ATOM 748 0 TRP 124 58.787 57.494 26.209 1.00 24.57 A C ATOM 748 0 TRP 124 58.787 57.494 26.209 1.00 24.57 A C ATOM 749 N ARG 125 58.013 58.218 27.013 1.00 24.36 A N ATOM 750 CA ARG 125 56.189 58.612 28.609 1.00 23.36 A C ATOM 751 CB ARG 125 56.189 58.621 28.609 1.00 23.36 A C ATOM 752 CC ARG 125 56.189 58.621 28.609 1.00 23.36 A C ATOM 755 CZ ARG 125 56.995 59.599 129 23.385 A C ATOM 756 NIL ARG 125 55.090 59.579 31.269 1.00 24.37 A C ATOM 757 NIL2 ARG 125 55.090 59.579 31.269 1.00 22.381 A C ATOM 756 NIL ARG 125 56.051 59.857 33.347 1.00 24.42 A N ATOM 757 NIL2 ARG 125 55.993 58.605 29.308 1.00 23.36 A C ATOM 756 NIL ARG 125 56.051 59.357 33.347 1.00 24.42 A N ATOM 757 NIL2 ARG 125 56.051 59.357 33.347 1.00 24.42 A N ATOM 757 NIL2 ARG 125 55.090 59.579 31.269 1.00 25.99 A N A ATOM 757 NIL2 ARG 125 55.090 59.579 31.269 1.00 22.30 A N A ATOM 760 N HIS 126 55.6051 58.063 25.861 1.00 22.30 A N A ATOM 760 N HIS 126 55.861 58.063 25.867 20.20 20.00 23.33 A N A ATOM 760 N HIS 126 55.861 58.063 25.464 35.00 25.09 A N A ATOM 760 N HIS 126 55.861 58.063 25.474 1.00 24.40 A C ATOM 760 N HIS 126 55.861 58.063 25.444 1.00 24.40 A C ATOM 761 CA HIS 126 55.861 58.063 25.444 1.00 24.40 A C ATOM 760 N HIS 126 55.861 58.063 25.444 1.00 24.40 A C ATOM 760 N HIS 126 55.861 58.065 25.22 26.00 1.00 22.35 A C ATOM 760 N HIS 126 55.202 60.00 42.203 1.00 23.39 A N A ATOM 760 N HIS 126 55.861 55.202 60.00 42.20	ATOM	735 N								_	
ATOM 738 CG TRP 124 61.052 60.357 24.934 1.00 19.79 A C C ATOM 739 CD2 TRP 124 62.444 60.061 25.127 1.00 19.03 A C ATOM 740 CE2 TRP 124 63.175 60.913 24.270 1.00 19.13 A C C ATOM 741 CB3 TRP 124 63.175 60.913 24.270 1.00 19.13 A C C ATOM 742 CD1 TRP 124 60.999 61.350 24.006 1.00 18.84 A C ATOM 743 NE1 TRP 124 62.270 61.690 23.597 1.00 18.74 A N A N ATOM 744 C72 TRP 124 64.571 60.885 24.196 1.00 17.77 A C C ATOM 745 C73 TRP 124 64.573 59.185 24.996 1.00 17.77 A C C ATOM 746 CH2 TRP 124 65.229 59.886 24.996 1.00 17.77 A C C ATOM 746 CH2 TRP 124 65.295 59.896 24.996 1.00 17.07 A C ATOM 747 C TRP 124 58.490 56.350 25.861 1.00 25.71 A O C ATOM 748 0 TRP 124 58.490 56.350 25.861 1.00 24.35 A N A TOM 749 N ARG 125 58.013 58.218 27.013 1.00 24.35 A N A TOM 750 CA ARG 125 56.189 58.621 27.013 1.00 24.35 A N A TOM 750 CA ARG 125 56.189 58.601 28.809 1.00 23.36 A C ATOM 751 CB ARG 125 56.189 58.601 28.809 1.00 23.36 A C ATOM 753 CD ARG 125 56.935 58.065 29.308 1.00 23.36 A C C ATOM 755 CC ARG 125 56.935 58.065 29.308 1.00 23.85 A C ATOM 755 CC ARG 125 56.935 58.865 29.308 1.00 23.85 A C ATOM 755 CC ARG 125 55.090 59.579 31.269 1.00 25.99 A N A TOM 756 NH1 ARG 125 55.090 59.579 31.269 1.00 25.99 A N A ATOM 756 NH1 ARG 125 55.090 59.357 33.347 1.00 26.04 A C ATOM 757 NH2 ARG 125 55.090 59.357 33.347 1.00 24.40 A C ATOM 756 CA RG 125 55.006 57.324 26.541 1.00 24.00 A C ATOM 757 NH2 ARG 125 55.006 57.324 26.541 1.00 24.00 A C ATOM 760 N HIS 126 55.501 55.006 57.324 26.541 1.00 24.00 A C ATOM 760 N HIS 126 55.651 58.063 25.403 1.00 22.35 A N ATOM 765 ND HIS 126 52.997 59.301 22.357 1.00 25.094 A C ATOM 765 ND HIS 126 52.997 59.311 22.387 1.00 24.42 A N ATOM 765 ND HIS 126 55.409 57.800 24.403 1.00 22.48 A N A ATOM 765 ND HIS 126 55.651 58.063 22.400 1.00 22.35 A C ATOM 760 N HIS 126 55.651 58.063 22.400 1.00 22.35 A C ATOM 765 ND HIS 126 52.975 59.99 22.42 56.661 1.00 24.30 A N A ATOM 765 ND HIS 126 55.200 60.064 27.532 1.00 22.48 A N A ATOM 765 ND HIS 126 55.200 60.064 27.532 1.00 22.48 A N A ATOM 765 ND HIS 126 55.200 60.064	ATOM								-		
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ATOM 777 CA TYR 128 58.501 55.207 19.403 1.00 22.06 A C ATOM 778 CB TYR 128 57.787 53.962 19.928 1.00 21.99 A C ATOM 779 CG TYR 128 56.413 53.712 19.331 1.00 22.49 A C ATOM 780 CD1 TYR 128 55.257 54.112 20.003 1.00 23.20 A C ATOM 781 CE1 TYR 128 53.992 53.857 19.487 1.00 19.81 A C ATOM 782 CD2 TYR 128 56.267 53.049 18.109 1.00 20.70 A C								19.861			
ATOM 778 CB TYR 128 57.787 53.962 19.928 1.00 21.99 A C ATOM 779 CG TYR 128 56.413 53.712 19.331 1.00 22.49 A C ATOM 780 CD1 TYR 128 55.257 54.112 20.003 1.00 23.20 A C ATOM 781 CE1 TYR 128 53.992 53.857 19.487 1.00 19.81 A C ATOM 782 CD2 TYR 128 56.267 53.049 18.109 1.00 20.70 A C											
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ATOM 780 CD1 TYR 128 55. 257 54. 112 20. 003 1. 00 23. 20 A C ATOM 781 CE1 TYR 128 53. 992 53. 857 19. 487 1. 00 19. 81 A C ATOM 782 CD2 TYR 128 56. 267 53. 049 18. 109 1. 00 20. 70 A C		779	CG	TYR					1.00 22.49	y A	
ATOM 782 CD2 TYR 128 56.267 53.049 18.109 1.00 20.70 A C									1.00 23.20	J A 1 A	
ATUM 102 CD2 TTR 120 CD. 201 CD. 201 17 F20 1 00 20 27 A											
ATOM 783 CEZ TYK 128 55.007 52.791 17.580 1.00 20.67 A C											
	ATOM	783	CEZ	TYK	128	55.00	j 54. (91	14.000	1.00 40.0	• '	

SUBSTITUTE SHEET (RULE 26)

						(Continued)
		F	IG. 4-	17			
ATOM	784 CZ TYR	128 53.	872 53.197	18. 279	1.00 22.39	Α	С
ATOM		128 52.		17.776	1.00 19.88	Α	0
ATOM		128 58.	'		1.00 22.84	A	C
ATOM ATOM		128 57.			1.00 24.63	A	0
ATOM		129 59.		17.320	1.00 22.88	A	N
ATOM		129 59.		15.874	1.00 25.24	A	C
ATOM			723 54.474	15. 245	1.00 27.54	A	C
ATOM	791 OG1 THR		756 53.676	15.844	1.00 33.01	A	0
ATOM	792 CG2 THR	129 61.	025 55.951	15.419	1.00 28.79	A	C
ATOM	793 C THR	129 59.	062 52.675	15.580	1.00 24.85	A	C
ATOM	794 0 THR		168 51.811	16.457	1.00 22.29	A	O N
ATOM	795 N ALA		692 52.411	14. 337	1.00 24.54	A	C
ATOM	796 CA ALA		356 51.062	13.943	1.00 25.98	A	C
ATOM	797 CB ALA		061 50.636	14.618	1. 00 22. 73 1. 00 26. 81	A A	Č
ATOM	798 C ALA		195 50.983	12.445	1.00 20.01	A	Ö
ATOM	799 O ALA		277 51.988	11.740	1.00 27.32	A	N
ATOM	800 N SER		978 49.767	11.965 10.556	1.00 27.13	A	Ĉ
ATOM	801 CA SER		759 49.540	10. 059	1.00 28.58	Ä	č
ATOM	802 CB SER		643 48.403 995 48.822	10.033	1.00 29.90	Ä	Ö
ATOM	803 OG SER		995 48.822 290 49.187	10. 426	1.00 27.17	Ä	Ċ
ATOM	804 C SER		651 48.779	11.397	1.00 27.00	Ā	0
ATOM	805 O SER 806 N TYR		747 49.351	9. 232	1.00 27.56	Α	N
ATOM	806 N TYR 807 CA TYR		341 49.061	9. 029	1.00 28.28	A	C
ATOM ATOM	808 CB TYR		532 50.357	9.156	1.00 27.16	Α	С
ATOM	809 CG TYR		649 51.046	10.507	1.00 25.23	Α	С
ATOM	810 CD1 TYR		692 50.842	11.500	1.00 24.00	Α	C
ATOM	811 CE1 TYR	132 52	. 790 51. 483	12.735	1.00 23.00	A	C
ATOM	812 CD2 TYR		. 714 51. 908	10. 785	1.00 22.89	A	C
ATOM	813 CE2 TYR		. 822 52. 549	12.016	1.00 21.43	A	C
ATOM	814 CZ TYR			12.985	1.00 22.58	A	C
ATOM	815 OH TYR		. 940 52. 976	14. 198	1.00 21.69	A	C 0
ATOM	816 C TYR		. 071 48. 418		1.00 28.72 1.00 29.54	A A	0
ATOM	817 O TYR		. 794 48. 639		1.00 29.54	A	N
ATOM	818 N ASP		.028 47.604		1.00 29.99	A	C
ATOM	819 CA ASP		. 629 46. 956 . 147 45. 519		1.00 31.00	A	Č
ATOM	820 CB ASP				1.00 33.92	Ä	Č
ATOM	821 CG ASP		. 541 45. 436 . 773 46. 042		1.00 33.52	A	Ö
ATOM	822 OD1 ASP		i. 400 44. 756		1.00 35.83	A	0
ATOM	823 OD2 ASP 824 C ASP		.125 46.952		1.00 30.39	Α	C
ATOM	824 C ASP 825 O ASP). 467 46. 384		1.00 33.36	Α	0
ATOM ATOM	826 N ILE). 579 47. 598		1.00 28.05	Α	N
ATOM	827 CA ILE		0.144 47.652	5.157	1.00 25.68	A	Č
ATOM	828 CB ILE		3. 732 48. 816		1.00 23.81	A	C
ATOM	829 CG2 ILE		7. 221 48. 954	4. 289	1.00 22.12	A	C
ATOM	830 CG1 ILE		9.421 50.095	4.752		A	C
ATOM	831 CD1 ILE	134 49	9. 232 51. 277			A	C C
ATOM	832 C ILE	134 4	8. 635 46. 368	3 4.524	1.00 27.46	A	U
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				((Continued)
`			FIG. 4-18		
ATOM	833 0 ILE	134	49. 171 45. 894 3. 521 1. 00 27. 19	A	0 .
ATOM	834 N TYR	135	47, 599 45, 805 5, 127 1, 00 29, 43	A	N
ATOM	835 CA TYR	135	46, 985 44, 588 4, 628 1, 00 30, 54	A	C
ATOM	836 CB TYR	135	46, 800 43, 588 5, 772 1, 00 33, 25	Ą	C
ATOM	837 CG TYR	135	46. 276 42. 242 5. 343 1. 00 35. 66	A	C
ATOM	838 CD1 TYR	135	47. 113 41. 311 4. 731 1. 00 37. 89	A	C
ATOM	839 CE1 TYR	135	10.001 10.000	A	C
ATOM	840 CD2 TYR	135	11.303	A	C
ATOM	841 CE2 TYR	135	11, 111 10,000	A ^	C C
ATOM	842 CZ TYR	135	10. 200 00. 101	A A	Õ
ATOM	843 OH TYR	135	11.011 00.020	A	Č
ATOM.	844 C TYR	135	10.020	A	Õ
ATOM	845 0 TYR	135	11.010	A	N
ATOM	846 N ASP	136		Ä	Ċ
ATOM	847 CA ASP	136 136	44. 323 44. 857 0. 655 1. 00 32. 51	A	Č
ATOM	848 CB ASP 849 CG ASP	136		A	C
ATOM	849 CG ASP 850 OD1 ASP	136		Α	0
ATOM ATOM	851 OD2 ASP	136	10, 110	Α	0
ATOM	852 C ASP	136	43.019 43.797 2.549 1.00 35.55	Α	C
ATOM	853 0 ASP	136	42.822 42.810 1.846 1.00 36.12	Α	0 .
ATOM	854 N LEU	137	42.341 44.040 3.669 1.00 38.03	A	N
ATOM	855 CA LEU	137	11.000	A	C
ATOM	856 CB LEU	137	10. 110	A	C
ATOM	857 CG LEU	137	11.100	A	C
ATOM	858 CD1 LEU	137	40. 206 45. 257 7. 307 1. 00 37. 54	A A	C C
ATOM	859 CD2 LEU	137	41.686 43.243 7.286 1.00 38.91 40.392 42.536 3.134 1.00 42.88	A	Č
ATOM	860 C LEU	137		A	ŏ
ATOM	861 0 LEU	137	40. 038 41. 362 3. 225 1. 00 43. 41 39. 997 43. 322 2. 141 1. 00 45. 42	Ä	Ň
ATOM	862 N ASN 863 CA ASN	138 138	39. 132 42. 796 1. 093 1. 00 48. 50	Ä	Ċ
ATOM	863 CA ASN 864 CB ASN	138	38. 537 43. 936 0. 264 1. 00 49. 71	A	C
ATOM	865 CG ASN	138	37. 127 44. 291 0. 697 1. 00 50. 83	Α	С
ATOM ATOM	866 OD1 ASN	138	36.873 44.555 1.871 1.00 51.97	Α	0
ATOM	867 ND2 ASN	138	36. 202 44. 296 -0. 254 1. 00 52. 74	Α	N
ATOM	868 C ASN	138	39. 884 41. 824 0. 191 1. 00 49. 47	A	C
ATOM	869 0 ASN	138	39.642 40.619 0.240 1.00 50.62	Α	0
ATOM	870 N LYS	139	40.794 42.346 -0.626 1.00 50.26	A	N
ATOM	871 CA LYS	139	41.581 41.507 -1.526 1.00 51.09	A	C
ATOM	872 CB LYS	139	42.510 42.374 -2.382 1.00 51.15	A	C C
ATOM	873 CG LYS		41. 785 43. 427 -3. 212 1. 00 53. 38 42. 753 44. 331 -3. 974 1. 00 54. 25	A A	C
ATOM	874 CD LYS		70.100	A	C
ATOM	875 CE LYS		7 01 7 1 00 50 00	A	N
ATOM	876 NZ LYS		0 700 4 00 71 00	A	Č
ATOM	877 C LYS		42.413 40.528 -0.703 1.00 51.63 43.148 39.708 -1.251 1.00 51.80	Ä	Ŏ
ATOM	878 0 LYS		42. 288 40. 624 0. 618 1. 00 51. 49	Ä	Ň
ATOM ATOM	879 N ARG 880 CA ARG		43.025 39.768 1.534 1.00 51.71	Ā	C
ATOM	881 CB ARG		42.338 38.408 1.642 1.00 53.88	Α	C
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		(Continued)
FIG. 4-19		
ATOM 883 CD ARG 140 40. 257 37. 128 2. 211 1. ATOM 884 NE ARG 140 40. 936 36. 235 3. 142 1. ATOM 885 CZ ARG 140 40. 633 34. 950 3. 294 1.	00 57.36 A 00 60.02 A 00 62.76 A 00 64.87 A 00 66.83 A	C C N C N
ATOM 887 NH2 ARG 140 41.298 34.206 4.169 1. ATOM 888 C ARG 140 44.464 39.603 1.066 1.	00 65.62 A 00 50.29 A	N C
ATOM 890 N GLN 141 45.096 40.723 0.741 1.	. 00 50. 21 A . 00 49. 82 A . 00 48. 70 A	O N C
ATOM 892 CB GLN 141 46.487 40.815 -1.260 1.	. 00 48. 70 A . 00 50. 32 A . 00 55. 02 A	C C
ATOM 894 CD GLN 141 47.640 40.179 -3.413 1. ATOM 895 OE1 GLN 141 48.582 39.756 -4.088 1.	. 00 57. 33 A . 00 57. 97 A	C 0
ATOM 897 C GLN 141 47.293 41.837 0.898 1.	. 00 58. 85 A . 00 46. 02 A . 00 45. 33 A	N C O
ATOM 899 N LEU 142 48.594 41.610 1.013 1. ATOM 900 CA LEU 142 49.505 42.578 1.605 1.	. 00 43. 34 A . 00 41. 50 A	N C
ATOM 902 CG LEU 142 51.489 42.501 3.359 1.	. 00 41. 17 A . 00 42. 33 A . 00 42. 24 A	C C C
ATOM 904 CD2 LEU 142 52.254 43.677 2.772 1.	.00 42.24 A .00 42.66 A .00 40.87 A	C C
ATOM 906 0 LEU 142 50.557 43.030 -0.506 1. ATOM 907 N ILE 143 49.978 44.806 0.748 1.	. 00 41. 57 A . 00 39. 20 A	0 N
ATOM 909 CB ILE 143 49.921 47.202 0.104 1.	. 00 37.17 A . 00 36.58 A . 00 35.56 A	C C
ATOM 911 CG1 ILE 143 48.398 47.197 0.030 1. ATOM 912 CD1 ILE 143 47.777 48.494 0.468 1.	. 00 34. 64 A . 00 37. 28 A	C C
ATOM 914 0 ILE 143 52.603 45.859 0.849 1.	. 00 36. 06 A . 00 36. 63 A . 00 35. 40 A	C O N
ATOM 916 CA THR 144 54.046 45.933 -1.459 1. ATOM 917 CB THR 144 54.616 44.654 -2.124 1.	. 00 35. 79 A . 00 35. 59 A	C C
ATOM 919 CG2 THR 144 54.121 43.415 -1.403 1.	. 00 37. 13 A . 00 33. 21 A . 00 35. 43 A	0 C C
ATOM 921 0 THR 144 55.700 47.311 -2.511 1. ATOM 922 N GLU 145 53.577 48.015 -2.602 1.	. 00 36. 45 A . 00 36. 27 A	O N
ATOM 923 CA GLU 145 53.891 49.214 -3.369 1. ATOM 924 CB GLU 145 52.962 49.297 -4.586 1.	. 00 36. 32 A . 00 38. 36 A . 00 42. 66 A	C C
ATOM 926 CD GLU 145 54.667 49.639 -6.418 1.	. 00 42. 66 A . 00 45. 91 A . 00 45. 49 A	C O
ATOM 928 OE2 GLU 145 54.456 50.283 -7.476 1. ATOM 929 C GLU 145 53.775 50.496 -2.544 1.	. 00 45. 56 A . 00 35. 06 A . 00 34. 22 A	0 C 0

		FIG. 4-20	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	931 N GLU 146 932 CA GLU 146 933 CB GLU 146 934 CG GLU 146 935 CD GLU 146 936 OE1 GLU 146 937 OE2 GLU 146 938 C GLU 146 939 O GLU 146 940 N ARG 147 941 CA ARG 147 942 CB ARG 147 942 CB ARG 147 944 CD ARG 147 945 NE ARG 147 946 CZ ARG 147 947 NH1 ARG 147 947 NH1 ARG 147 948 NH2 ARG 147 949 C ARG 147 950 O ARG 147 951 N ILE 148 952 CA ILE 148 953 CB ILE 148 953 CB ILE 148 954 CG2 ILE 148 955 CG1 ILE 148 955 CG1 ILE 148 956 CD1 ILE 148 957 C ILE 148 956 CD1 ILE 148 957 C ILE 148 956 CD1 ILE 148 957 C ILE 148 958 O ILE 148 956 CD1 ILE 148 956 CD1 ILE 148 957 C ILE 148 956 CD1 ILE 148 956 CD1 ILE 148 957 C ILE 148 956 CD1 ILE 148 957 C ILE 148 958 O ILE 148 959 N PRO 149 960 CD PRO 149 961 CA PRO 149 962 CB PRO 149 963 CG PRO 149 964 C PRO 149 965 O PRO 149 966 N ASN 150 967 CA ASN 150 967 CA ASN 150 970 OD1 ASN 150 971 ND2 ASN 150 971 ND2 ASN 150	54. 692 51. 428 -2. 782 1. 00 33. 82 54. 699 52. 706 -2. 079 1. 00 32. 54 53. 594 53. 608 -2. 630 1. 00 33. 84 53. 708 53. 924 -4. 107 1. 00 33. 18 54. 992 54. 651 -4. 455 1. 00 32. 11 55. 677 55. 129 -3. 528 1. 00 32. 11 55. 309 54. 754 -5. 660 1. 00 35. 19 54. 495 52. 521 -0. 579 1. 00 32. 26 53. 644 53. 172 0. 031 1. 00 32. 38 55. 287 51. 638 0. 013 1. 00 30. 84 55. 185 51. 357 1. 437 1. 00 29. 94 55. 992 50. 107 1. 774 1. 00 31. 91 55. 376 48. 821 1. 262 1. 00 33. 35 55. 999 47. 649 1. 963 1. 00 37. 64 58. 271 46. 812 2. 356 1. 00 39. 76 57. 844 46. 143 3. 421	A A A A A A A A A A A A A A A A A A A
ATOM ATOM ATOM ATOM ATOM ATOM	974 N ASN 151 975 CA ASN 151 976 CB ASN 151 977 CG ASN 151 978 OD1 ASN 151 979 ND2 ASN 151	61. 387 53. 022 10. 208 1. 00 28. 46 61. 734 54. 078 11. 154 1. 00 28. 87 63. 137 54. 622 10. 877 1. 00 30. 74 64. 213 53. 571 11. 048 1. 00 34. 06 64. 360 52. 678 10. 219 1. 00 36. 24 64. 965 53. 666 12. 139 1. 00 37. 62	A N A C A C A C A O A N
111 0111			

					(Continued)
				FIG. 4-21	·
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	981 982 983 984 985 986 987 988 990 991 992 993 994 995 996 997 998 999 1000 1001 1002 1003 1004 1005 1006 1007	C ASN O ASN N THR CA THR CB THR OG1 THR CG2 THR C THR N GLN CA GLN CA GLN CA GLN CB GLN CB GLN CCB CD GLN CCB CD CD CD CCB TRP	151 151 152 152 152 152 153 153 153 153 153 154 154 154 154 154 154	60. 734 55. 230 11. 111 1. 00 28. 16 61. 118 56. 400 11. 112 1. 00 28. 85 59. 450 54. 895 11. 064 1. 00 26. 20 58. 415 55. 911 11. 041 1. 00 24. 74 57. 119 55. 389 10. 399 1. 00 25. 27 57. 351 55. 125 9. 009 1. 00 24. 18 56. 004 56. 426 10. 538 1. 00 23. 99 58. 139 56. 319 12. 474 1. 00 23. 46 57. 933 55. 476 13. 340 1. 00 25. 16 58. 134 57. 620 12. 721 1. 00 22. 30 57. 916 58. 129 14. 063 1. 00 20. 67 58. 501 59. 534 14. 161 1. 00 19. 09 60. 022 59. 543 13. 906 1. 00 13. 74 60. 495 60. 853 13. 331 1. 00 14. 57 60. 089 61. 260 12. 233 1. 00 12. 70 61. 375 61. 524 14. 0	A C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C C A A C C C C A A C C C C A A C C C C A A C C C C A A C C C C A C C C C A C C C C A C C C C A C C C C C A C
ATOM ATOM ATOM	1008 1009 1010	CZ2 TRP CZ3 TRP CH2 TRP C TRP O TRP	154 154 154 154 154	51. 263 57. 339 17. 847 1. 00 22. 07 49. 897 57. 656 17. 784 1. 00 23. 43 53. 291 58. 054 12. 576 1. 00 21. 43 53. 642 58. 572 11. 518 1. 00 22. 33	A C A C A C A O
ATOM ATOM ATOM ATOM	1011 1012 1013 1014 1015	N VAL CA VAL CB VAL CG1 VAL	155 155 155 155	52. 173 57. 343 12.703 1. 00 21. 97 51. 267 57. 103 11. 579 1. 00 20. 81 51. 642 55. 797 10. 840 1. 00 19. 96 51. 835 54. 687 11. 842 1. 00 21. 34	A N A C A C A C
ATOM ATOM ATOM ATOM ATOM	1016 1017 1018 1019	CG2 VAL C VAL O VAL N THR	155 155 155 156	50. 562 55. 414 9. 833 1. 00 20. 23 49. 840 57. 004 12. 104 1. 00 21. 39 49. 601 56. 425 13. 162 1. 00 21. 74 48. 898 57. 576 11. 364 1. 00 20. 70	A C . A C A O A N
ATOM ATOM ATOM ATOM ATOM	1020 1021 1022 1023 1024	CA THR CB THR OG1 THR CG2 THR C THR O THR	156 156 156 156 156 156	47. 504 57. 557 11. 768 1. 00 21. 67 47. 189 58. 736 12. 716 1. 00 22. 79 45. 771 58. 848 12. 890 1. 00 25. 50 47. 707 60. 031 12. 145 1. 00 22. 46 46. 558 57. 633 10. 577 1. 00 22. 20 46. 861 58. 276 9. 577 1. 00 22. 72	A C A C A C A C A C A C
ATOM ATOM ATOM ATOM	1025 1026 1027 1028	N TRP CA TRP CB TRP	157 157 157	45. 413 56. 966 10. 689 1. 00 21. 38 44. 423 56. 985 9. 627 1. 00 21. 45 43. 426 55. 825 9. 765 1. 00 21. 88	A N A C A C

					FΙ	G. 4	- 22			(Continued)
ATOM ATOM ATOM ATOM ATOM	1029 1030 1031 1032 1033	CG 1 CD2 1 CE2 1 CE3 1 CD1 1	TRP TRP TRP	157 157 157 157 157	43. 995 44. 315 44. 843 44. 208 44. 328	54. 450 53. 800 52. 531 54. 168 53. 571	9. 599 8. 364 8. 686 7. 019 10. 592	1.00 20.88 1.00 18.96 1.00 19.67 1.00 17.93 1.00 20.82	A A A A	C C C C
ATOM ATOM ATOM ATOM ATOM	1034 1035 1036 1037 1038	NE1 7 CZ2 7 CZ3 7 CH2 7 C	TRP TRP TRP TRP TRP	157 157 157 157 157 157	44. 838 45. 265 44. 627 45. 149 43. 650 43. 750	52. 417 51. 626 53. 267 52. 011 58. 276 58. 917	10. 052 7. 708 6. 046 6. 397 9. 801 10. 843	1.00 21.01 1.00 19.12 1.00 19.76 1.00 19.30 1.00 23.03 1.00 25.03	A A A A A	N C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM	1039 1040 1041 1042 1043 1044	N S CA S CB S OG S C	SER SER SER SER SER	158 158 158 158 158	42. 889 42. 064 41. 667 41. 208 40. 845	58. 663 59. 855 60. 362 59. 311 59. 377	8. 784 8. 889 7. 502 6. 679 9. 678	1.00 23.17 1.00 23.44 1.00 22.82 1.00 23.84 1.00 23.86	A A A A	N C C O C
ATOM ATOM ATOM ATOM ATOM ATOM	1045 1046 1047 1048 1049 1050	N I CD I CA I CB I CG I	PRO PRO PRO PRO PRO	158 159 159 159 159 159	40. 613 40. 056 40. 136 38. 876 38. 270 39. 427	58. 176 60. 301 61. 762 59. 922 61. 264 62. 214	9. 781 10. 247 10. 114 11. 029 11. 419 11. 353	1.00 24.35 1.00 24.17 1.00 24.24 1.00 23.40 1.00 23.45 1.00 24.19	A A A A A	O N C C C
ATOM ATOM ATOM ATOM ATOM ATOM	1051 1052 1053 1054 1055 1056	O I N V CA V	PRO VAL VAL VAL	159 159 160 160 160 160	37. 901 37. 191 37. 878 36. 977 35. 784 35. 066	59. 090 58. 248 59. 334 58. 640 59. 545 59. 064	10. 224 10. 771 8. 919 8. 014 7. 689 6. 449	1.00 25.36 1.00 27.14 1.00 25.28 1.00 23.99 1.00 24.54 1.00 26.50	A A A A A	C O N C C C
ATOM ATOM ATOM ATOM ATOM ATOM	1057 1058 1059 1060 1061 1062	CG2 Y C Y O Y N C CA C	VAL VAL VAL	160 160 160 161 161 161	34. 834 37. 679 38. 570 37. 268 37. 876 39. 121	59. 559 58. 218 58. 908 57. 080 56. 579 55. 786	8. 875 6. 730 6. 245 6. 181 4. 962 5. 286	1.00 26.15 1.00 23.78 1.00 24.51 1.00 24.05 1.00 22.93 1.00 23.87	A A A A A	C C O N C C
ATOM ATOM ATOM ATOM ATOM	1063 1064 1065 1066 1067	O O N I CA I CB I CG I	GLY HIS HIS HIS HIS	161 162 162 162 162	39. 144 40. 164 41. 423 41. 419 41. 075	55. 045 55. 950 55. 239 53. 923 54. 087	6. 269 4. 476 4. 695 3. 920 2. 475	1.00 24.24 1.00 25.01 1.00 25.86 1.00 26.04 1.00 27.52	A A A A	O N C C C
ATOM ATOM ATOM ATOM ATOM ATOM	1068 1069 1070 1071 1072 1073	0 1	HIS HIS HIS HIS HIS	162 162 162 162 162 162	41.614 40.039 39.956 40.900 42.660 43.636	54. 875 53. 402 53. 764 54. 656 56. 053 55. 501	1. 515 1. 874 0. 606 0. 363 4. 305 3. 794	1.00 27.58 1.00 27.77 1.00 28.51 1.00 28.82 1.00 25.44 1.00 24.38	A A A A A	C N C N C
ATOM ATOM ATOM ATOM	1074 1075 1076 1077	CA 1	LYS LYS LYS LYS	163 163 163 163	42. 609 43. 751 43. 372 42. 528	57. 364 58. 221 59. 701 60. 216	4. 527 4. 224 4. 273 3. 130	1.00 24.47 1.00 23.45 1.00 21.75 1.00 21.55	A A A	N C C C

									(Continued)
				FIG	. 4 -	23			
ATOM	1078	CD LYS	163	42. 281	61. 706	3. 335	1.00 20.23	Α	С
ATOM	1079	CE LYS	163		32. 316	2. 228	1.00 18.07	Α	С
ATOM	1080	NZ LYS	163		33. 778	2.422	1.00 20.95	Α	N
ATOM	1081	C LYS	163		57. 961	5.309	1.00 23.44	Α	С
ATOM	1082	0 LYS	163	44. 425	57. 600	6.433	1.00 23.42	Α	0
ATOM	1083	N LEU	164	46.053	58. 146	4.979	1.00 23.11	Α	N
ATOM	1084	CA LEU	164	47.117	57. 937	5.950	1.00 23.65	Α	С
ATOM	1085	CB LEU	164	48.014	56. 773	5.524	1.00 24.35	A _.	С
ATOM	1086	CG LEU	164		55. 351	5.848	1.00 25.57	Α	C
ATOM	1087	CD1 LEU	164		54. 349	5.219	1.00 25.59	A	C
ATOM	1088	CD2 LEU	164		55.162	7.359	1.00 25.62	A	Č
ATOM	1089	C LEU	164		59. 182	6.120	1.00 23.21	A	C
ATOM	1090	0 LEU	164		59. 943	5.177	1.00 24.34	A	0
ATOM	1091	N ALA	165		59. 383	7. 335	1.00 21.88	A	N
ATOM	1092	CA ALA	165		50. 508	7.649	1.00 21.58	A	C
ATOM	1093	CB ALA	165		51. 583	8. 376	1.00 21.77	A	C
ATOM	1094	C ALA	165		59. 953	8. 545	1.00 22.07	A	C
ATOM	1095	0 ALA	165		59. 285	9.537	1.00 22.91	A	0
ATOM	1096	N TYR	166		60. 208	8. 201	1.00 22.02	A	N
ATOM	1097	CA TYR	166		59. 697		1.00 21.73	A	C
ATOM	1098	CB TYR	166		58. 319		1.00 22.38	A	C
ATOM	1099	CG TYR	166		58. 315	7. 141	1.00 22.11	A	C
ATOM	1100	CD1 TYR	166		58. 661	6.964	1.00 21.28	A	C
ATOM	1101	CE1 TYR	166		58. 638	5. 704	1.00 22.05	A	C
ATOM	1102	CD2 TYR	166		57. 949	6.015	1.00 20.67	A	C
ATOM	1103	CE2 TYR	166		57. 923	4. 753	1.00 20.02	A	C C
ATOM	1104	CZ TYR	166		58. 268	4.603	1.00 21.75	A	0
ATOM	1105	OH TYR	166		58. 252	3. 352 9. 057	1.00 20.77 1.00 21.64	A A	C
ATOM	1106	C TYR	166		60. 643 61. 464	8. 157	1.00 21.04	A	0
ATOM	1107	O TYR	166 167		60. 529	10.111	1.00 21.01	A	N
ATOM	1108	N VAL CA VAL	167		61.371	10. 111	1.00 20.28	A	Č
ATOM ATOM	1109 1110	CA VAL	167		62.011	11.644	1.00 19.10	Ä	C
ATOM	1111	CG1 VAL	167		62. 984	11.731	1.00 18.58	A	č
ATOM	11112	CG2 VAL	167		62. 713	11. 916	1.00 18.36	A	č
ATOM	1113	C VAL	167		60. 537		1.00 20.06	Ä	č
ATOM		0 VAL					1.00 21.80	Ä	
ATOM	1115	N TRP	168		61.023	9. 233	1.00 19.65	A	Ň
ATOM	1116	CA TRP	168		60. 320	8. 964	1.00 19.61	Ä	Ĉ
ATOM	1117	CB TRP	168		59. 558	7.646	1.00 20.07	Ä	Č
ATOM	1118	CG TRP	168		58. 772	7. 353	1.00 23.12	A	Ċ
ATOM	1119	CD2 TRP	168		59.011	6. 300	1.00 21.38	Α	C
ATOM	1120	CE2 TRP	168		58. 061	6.436	1.00 21.58	Α	C
ATOM	1121	CE3 TRP	168		59. 936	5. 256	1.00 21.74	Α	Ċ
ATOM	1122	CD1 TRP	168		57. 712	8.066	1.00 22.86	Α	C
ATOM	1123	NE1 TRP	168		57. 281	7. 521	1.00 21.54	Α	N
ATOM	1124	CZ2 TRP	168		58.012	5.563	1.00 23.71	Α	С
ATOM	1125	CZ3 TRP	168		59.889	4.386	1.00 23.21	Α	С
ATOM	1126	CH2 TRP	168		58. 934	4.546	1.00 22.74	Α	С

			(Continued)
		FIG. 4-25	(002232222
ATOM 1177 CG ATOM 1178 C ATOM 1179 O ATOM 1180 N ATOM 1181 CA ATOM 1182 CE ATOM 1183 CG ATOM 1184 CI ATOM 1185 CG ATOM 1186 NZ ATOM 1187 C ATOM 1188 O ATOM 1187 C ATOM 1189 N ATOM 1190 CG ATOM 1191 CG ATOM 1191 CG ATOM 1193 CG ATOM 1194 CG ATOM 1195 CG ATOM 1196 O ATOM 1197 N ATOM 1198 CG ATOM 1198 CG ATOM 1199 CG ATOM 1199 CG ATOM 1199 CG ATOM 1201 CG ATOM 1202 CG A	B LYS 175 G LYS 175 G LYS 175 D LYS 175 E LYS 175 LYS 175 LYS 175 LYS 175 LYS 175 LYS 176 B ILE 176 B ILE 176 GI ILE 177 CG GLU 177 CB GLU 177 CB GLU 177 CB GLU 177 CB GLU 177 CC GLU 177	48. 658 56. 125 -4. 456 1. 00 24. 86	A A A A A A A A A A A A A A A A A A A
	CG LEU 180	5 070 5 000 1 00 95 07	A C

ATOM 1225 CDI LEU 180						`				(Continued)
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ATOM 1262 NH2 ARG 184 62.170 66.853 3.506 1.00 20.35 A N ATOM 1263 C ARG 184 54.736 66.779 1.820 1.00 14.10 A C ATOM 1264 O ARG 184 54.569 67.650 0.972 1.00 14.71 A O ATOM 1265 N ILE 185 54.390 66.937 3.089 1.00 15.27 A N ATOM 1266 CA ILE 185 53.804 68.175 3.572 1.00 14.44 A C ATOM 1267 CB ILE 185 52.786 67.884 4.692 1.00 16.20 A C ATOM 1268 CG2 ILE 185 52.091 69.175 5.115 1.00 14.78 A C										
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ATOM 1265 N ILE 185 54.390 66.937 3.089 1.00 15.27 A N ATOM 1266 CA ILE 185 53.804 68.175 3.572 1.00 14.44 A C ATOM 1267 CB ILE 185 52.786 67.884 4.692 1.00 16.20 A C ATOM 1268 CG2 ILE 185 52.091 69.175 5.115 1.00 14.78 A C									_	
ATOM 1266 CA ILE 185 53.804 68.175 3.572 1.00 14.44 A C ATOM 1267 CB ILE 185 52.786 67.884 4.692 1.00 16.20 A C ATOM 1268 CG2 ILE 185 52.091 69.175 5.115 1.00 14.78 A C								1.00 15.27	A	N
ATOM 1267 CB ILE 185 52.786 67.884 4.692 1.00 16.20 A C ATOM 1268 CG2 ILE 185 52.091 69.175 5.115 1.00 14.78 A C								1.00 14.44	Α	
ATOM 1268 CG2 ILE 185 52.091 69.175 5.115 1.00 14.78 A C							4. 692		Α	
					52. 091	69. 175				
	ATOM	1269					4. 202	1.00 15.25	A	C
ATOM 1270 CD1 ILE 185 51.021 67.250 2.947 1.00 12.00 A C										
ATOM 1271 C ILE 185 54.847 69.172 4.091 1.00 14.33 A C										
ATOM 1272 0 ILE 185 54.647 70.377 3.994 1.00 14.95 A 0										
ATOM 1273 N THR 186 55.950 68.676 4.646 1.00 14.38 A N	ATOM	1273	N I	THR 186	55. 950	68.676	4. 646	1.00 14.38	. А	Ŋ

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				FΙ	G. 4	- 27			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1277 CC 1278 C 1279 O 1280 N 1281 CA 1282 CE 1283 CC 1284 CI 1285 CE 1286 CE 1287 CI 1288 NE 1289 CC 1290 CC 1291 CH 1292 C 1293 O 1294 N 1295 CA 1296 CE 1297 OC	B THR G1 THR G1 THR THR THR TRP A TRP B TRP C2 TRP E3 TRP E4 TRP E7 TRP E7 TRP E7 TRP E8 TRP E8 TRP E9 TRP E1 TRP	186 186 186 186 186 187 187 187 187 187 187 187 187 187 187	F I 56. 995 57. 051 57. 308 55. 734 58. 384 58. 643 59. 275 60. 655 60. 843 60. 392 59. 093 57. 829 61. 165 60. 392 57. 949 56. 692 57. 949 56. 692 56. 758 61. 607 62. 804 61. 077 61. 892 61. 122 59. 835 60. 955 62. 384 63. 198 61. 881 62. 296	69. 555 69. 549 68. 218 70. 060 69. 190 68. 055 70. 174 70. 020 70. 734 69. 949 69. 841 68. 954 70. 405 69. 149 68. 549 68. 616 70. 074 69. 185 70. 620 70. 725 70. 999 71. 605 72. 737 72. 253 73. 920 70. 642 71. 016 69. 412 68. 426	5. 169 6. 717 7. 181 7. 323 4. 663 4. 262 4. 696 4. 253 2. 915 1. 736 0. 135 1. 606 0. 941 -0. 020 -0. 597 0. 881 -0. 211 5. 292 5. 053 6. 449 7. 493 8. 180 8. 587 7. 232 9. 415 8. 552 9. 538	1. 00 15. 05 1. 00 15. 72 1. 00 18. 48 1. 00 13. 92 1. 00 17. 06 1. 00 19. 33 1. 00 18. 28 1. 00 16. 04 1. 00 13. 96 1. 00 14. 75 1. 00 15. 37 1. 00 15. 22 1. 00 12. 92 1. 00 12. 92 1. 00 17. 91 1. 00 16. 75 1. 00 17. 84 1. 00 15. 71 1. 00 19. 54 1. 00 11. 35 1. 00 11. 35 1. 00 11. 04 1. 00 9. 11 1. 00 9. 49 1. 00 14. 44 1. 00 9. 49 1. 00 14. 44 1. 00 16. 08	A A A A A A A A A A A A A A A A A A A	Continued) C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1303 C 1304 0 1305 N 1306 C 1307 CE 1308 CC 1309 CI 1310 CE 1311 NZ 1312 C 1313 0 1314 N 1315 C 1316 CI 1317 CC 1318 CI 1318 CI 1319 OB	GLY GLY LYS A LYS B LYS G LYS D LYS E LYS LYS LYS GLU A GLU B GLU G GLU E1 GLU GLU GLU	189 189 190 190 190 190 190 190 190 19	63. 794 64. 584 64. 196 65. 612 66. 189 67. 679 68. 181 69. 698 70. 207 65. 799 65. 384 66. 426 66. 674 67. 796 67. 894 69. 018 68. 970 69. 952 67. 015 67. 930	68. 421 68. 685 68. 117 68. 096 69. 512 69. 588 70. 997	9. 782 8. 881 11. 004 11. 346 11. 264 11. 472 11. 256	1.00 15.86 1.00 17.65 1.00 17.28 1.00 18.87 1.00 20.03 1.00 22.58 1.00 27.62 1.00 31.27 1.00 35.57 1.00 18.41 1.00 19.79 1.00 21.70 1.00 23.41 1.00 29.95 1.00 30.89 1.00 33.70 1.00 33.21 1.00 21.53 1.00 22.21	A A A A A A A A A A A A A A A A A A A	C O N C C C C C O O C O C O

									(Continued)
				FI	G. 4 -	- 29			
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1375 CG1 1376 CD1 1377 C 1378 O 1379 N 1380 CA 1381 CB 1382 OG1 1383 CG2 1384 C 1385 O 1386 N 1387 CA 1388 CB 1389 CG 1390 OD1 1391 OD2 1392 C 1393 O 1394 N 1395 CA 1396 CB 1397 CG 1398 CD2 1400 CE3 1401 CD1 1402 NE1	ILE ILE ILE ILE ILE ILE ILE ITHR THR THR THR THR THR THR THR THR TTHR TTRP TRP TRP TRP TRP TRP TTRP T	198 198 198 198 198 198 199 199 199 199	55. 378 56. 425 55. 874 57. 724 58. 798 55. 946 56. 507 55. 809 56. 264 55. 374 55. 462 53. 924	65. 097 63. 991 63. 013 64. 602 63. 565 66. 057 67. 091 65. 700 66. 547 66. 316 64. 944 66. 619 66. 334 65. 325 67. 301 67. 193 68. 576 69. 446 69. 190 70. 403 66. 515 66. 118 66. 381 65. 699 64. 679 64. 679 64. 953 66. 799 63. 661	16. 298 16. 011 14. 987 15. 494 15. 214 17. 318 16. 966 18. 583 19. 672 20. 908 21. 301 20. 583 20. 076 19. 734 20. 801 21. 289 21. 418 22. 491 22. 873 22. 945 22. 641 22. 999 23. 395 24. 672 25. 326 26. 510 27. 828 28. 564 28. 456 26. 507 27. 733 29. 897	1. 00 16. 59 1. 00 18. 21 1. 00 18. 51 1. 00 17. 86 1. 00 19. 35 1. 00 15. 95 1. 00 15. 42 1. 00 16. 68 1. 00 17. 40 1. 00 18. 82 1. 00 15. 72 1. 00 16. 00 1. 00 16. 12 1. 00 16. 12 1. 00 16. 87 1. 00 15. 49 1. 00 15. 49 1. 00 14. 82 1. 00 17. 16 1. 00 16. 41 1. 00 15. 97 1. 00 15. 54 1. 00 17. 01 1. 00 13. 14 1. 00 14. 90 1. 01 15. 25 1. 00 13. 65 1. 00 13. 65 1. 00 13. 65 1. 00 13. 64 1. 00 14. 03	A A A A A A A A A A A A A A A A A A A	CCCCCONCCOCCONCCCOOCONCCCCCCNC
ATOM ATOM ATOM	1404 CZ3	3 TRP 2 TRP	201 201 201	60. 502 60. 601 59. 529	66.009 64.797 66.327	29. 778 30. 486 25. 662	1.00 12.04 1.00 14.87 1.00 14.42	A A A	C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1407 0 1408 N 1409 CA 1410 CB 1411 CG	TRP VAL VAL VAL I VAL 2 VAL	201 202 202 202 202 202 202 202 202 203 203	58. 635 59. 691 58. 830 59. 402 59. 010 58. 947 57. 365 56. 497 57. 072 55. 676 55. 556 55. 227	65. 656 67. 615 68. 265 69. 639 70. 716 69. 963 68. 401 68. 404 68. 518 68. 606 69. 078 70. 542	26. 175 25. 931 26. 911 27. 330 26. 322 28. 753 26. 518 27. 391 25. 226 24. 805 23. 354 23. 227	1. 00 13. 63 1. 00 15. 14 1. 00 14. 23 1. 00 12. 99 1. 00 11. 02 1. 00 8. 71 1. 00 15. 76 1. 00 18. 74 1. 00 15. 58 1. 00 14. 25 1. 00 12. 35	A A A A A A A A A	0 N C C C C O N C C
ATOM ATOM		1 TYR 1 TYR	203 203	56. 231 55. 920	71. 508 72. 867	23. 193 23. 108	1.00 11.91 1.00 11.20	A A	C C

				710 4 20	(C	ontinued)
				FIG. 4-30		
ATOM	1421	CD2 TYR	203	53. 902 70. 966 23. 177 1. 00 12. 17 A		
ATOM	1422	CE2 TYR	203	53. 579 72. 314 23. 099 1. 00 10. 57 A 54. 588 73. 259 23. 061 1. 00 9. 67 A	_	5
ATOM	1423	CZ TYR	203			j .
ATOM	1424	OH TYR	$\begin{array}{c} 203 \\ 203 \end{array}$	54. 259 74. 586 22. 970 1. 00 7. 05 A 55. 024 67. 234 24. 951 1. 00 14. 92 A		Č
ATOM	1425	C TYR O TYR	203	53. 896 67. 124 25. 406 1. 00 15. 28 A		Ö
ATOM ATOM	1426 1427	N GLU	204	55. 744 66. 185 24. 570 1. 00 16. 35 A	Ì	V.
ATOM	1428	CA GLU	204	55. 222 64. 826 24. 684 1. 00 16. 96 A	. (C
ATOM	1429	CB GLU	204	56. 238 63. 812 24. 130 1. 00 14. 28 A		C
ATOM	1430	CG GLU	204	55. 928 62. 380 24. 540 1. 00 14. 97 A		C
ATOM	1431	CD GLU	204	56. 872 61. 345 23. 947 1. 00 19. 54 A		C 0
ATOM	1432	OE1 GLU	204	56. 697 60. 144 24. 271 1. 00 18. 49 A 57. 778 61. 714 23. 160 1. 00 18. 73 A		0
ATOM	1433	OE2 GLU	204	011110		C
ATOM	1434	C GLU O GLU	204 204	54. 868 64. 431 26. 128 1. 00 18. 02 A 53. 816 63. 848 26. 388 1. 00 17. 48 A		Õ
ATOM ATOM	1435 1436	O GLU N GLU	205	55. 757 64. 761 27. 059 1. 00 18. 67 A		N
ATOM	1437	CA GLU	205	55. 589 64. 409 28. 459 1. 00 20. 30 A		C
ATOM	1438	CB GLU	205	56. 970 64. 250 29. 096 1. 00 20. 92 A		C
ATOM	1439	CG GLU	205	56. 958 64. 035 30. 592 1. 00 24. 62 A		C
ATOM	1440	CD GLU	205	56. 563 62. 625 30. 974 1. 00 28. 17 A		C
ATOM	1441	OE1 GLU	205	56. 398 62. 355 32. 182 1. 00 32. 15 A 56. 424 61. 778 30. 069 1. 00 31. 11 A		0 0
ATOM	1442	OE2 GLU	205			C
ATOM	1443	C GLU O GLU	205 205	54.760 65.362 29.319 1.00 22.25 A 53.996 64.915 30.164 1.00 22.34 A		Ö
ATOM ATOM	1444 1445	O GLU N GLU	206	54. 902 66. 666 29. 107 1. 00 22. 70 A		N
ATOM	1446	CA GLU	206	54. 202 67. 632 29. 939 1. 00 23. 19 A	1	C
ATOM	1447	CB GLU	206	55. 203 68. 667 30. 453 1. 00 25. 39		C
ATOM	1448	CG GLU	206	56. 466 68. 088 31. 080 1. 00 27. 87		C
ATOM	1449	CD GLU	206	56. 188 67. 307 32. 345 1. 00 29. 45		C
ATOM	1450	OE1 GLU	206			0
ATOM	1451	OE2 GLU	206		l I	C
ATOM	1452	C GLU O GLU	206 206		į	Ö
ATOM ATOM	1453 1454	O GLU N VAL	207		À	N
ATOM	1455	CA VAL	207		A	C
ATOM	1456	CB VAL	207	52. 444 70. 235 26. 398 1. 00 25. 95	4	C
ATOM	1457	CG1 VAL	207		4	C
ATOM	1458	CG2 VAL	207	00. 100	4	C
ATOM	1459		207	00.001	A A	0 C
ATOM	1460		207		n A	N
ATOM	1461	N PHE	208 208		A	Č
ATOM ATOM	1462 1463		208		Ā	Č
ATOM	1464		208		A	C
ATOM	1465		208	51. 234 68. 911 22. 679 1. 00 29. 07	A	C
ATOM	1466		208	48.918 68.328 22.660 1.00 30.01	A	C
ATOM	1467	CE1 PHE	208	00.000	A	C
ATOM	1468		208	10.001	A A	C C
ATOM	1469	CZ PHE	208	49. 612 70. 464 21. 809 1. 00 30. 40	A	U

(Continued)

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ATOM	1470	С	PHE	208	50.082	65.163	25.506	1.00 26.13	A	Ç
ATOM	1471		PHE	208	49. 215	64.471	24.985	1.00 27.79	A	0
ATOM	1472	Ň	SER	209	50. 918	64.687	26.421	1.00 26.62	A	N
ATOM	1473	CA	SER	209	50. 852	63. 293	26.848	1.00 25.74	Α	С
			SER	209	49.645	63.059	27. 743	1.00 24.80	Α	С
ATOM	1474	CB			49. 871	63.629	29.014	1.00 29.47	Ä	0
ATOM	1475	OG	SER	209				1.00 25.50	Ä	č
ATOM	1476	C	SER	209	50.773	62.377	25. 642			ŏ
ATOM	1477	0	SER	209	50. 278	61.249	25. 716	1.00 25.72	A	
ATOM	1478	N	ALA	210	51.272	62.875	24. 524	1.00 23.72	A	N
ATOM	1479	CA	ALA	210	51.263	62.112	23. 299	1.00 22.80	A	C
ATOM	1480	CB	ALA	210	49. 977	62.364	22.530	1.00 20.62	A	Č
ATOM	1481	C	ALA	210	52. 455	62.560	22.492	1.00 21.87	Α	C
ATOM	1482	0	ALA	210	52. 986	63.644	22.703	1.0022.09	A	0
ATOM	1483	Ň	TYR	211	52.863	61.719	21.558	1.00 21.57	Α	N
ATOM	1484	CA	TYR	211	54.000	62.009	20.718	1.00 21.42	Α	С
	1485	CB	TYR	211	54. 725	60.711	20. 405	1.00 19.58	Α	C
ATOM				211	55. 921	60. 870	19.528	1.00 16.81	Ā	C
ATOM	1486	CG	TYR		56. 853	61.870	19.770	1.00 16.07	Ä	č
ATOM	1487	CD1	TYR	211	58. 002	61.971	19.001	1.00 18.18	Ä	č
ATOM	1488	CE1	TYR	211			18. 489	1.00 13.10	A	Č
ATOM	1489	CD2	TYR	211	56.160	59.976		1.00 17.31		Č
ATOM	1490	CE2	TYR	211	57. 306	60.065	17.716	-	A	C
ATOM	1491	CZ	TYR	211	58. 221	61.063	17.979	1.00 18.36	A	
ATOM	1492	OH	TYR	211	59. 360	61.149	17. 224	1.00 23.65	A	0
ATOM	1493	C	TYR	211	53. 588	62.689	19.428	1.00 22.96	A	C
ATOM	1494	0	TYR	211	54. 365	63. 443	18.837	1.00 25.79	A	0
ATOM	1495	N	SER	212	52.365	62.433	18.983	1.00 20.96	A	N
ATOM	1496	CA	SER	212	51.918	63.033	17.746	1.00 19.56	A	C
ATOM	1497	CB	SER	212	50. 835	62.175	17.090	1.00 20.97	A	С
ATOM	1498	0G	SER	212	49.635	62.208	17.829	1.00 21.79	Α	0
ATOM	1499	C	SER	212	51.397	64.439	17.959	1.00 18.50	A	C
ATOM	1500	Ö	SER	212	50. 933	64.789	19.040	1.00 16.31	A	0
ATOM	1501	Ň	ALA	213	51.493	65. 236	16.901	1.00 17.84	A	N
ATOM	1502	CA	ALA	213	51.036	66.610	16.903	1.00 16.02	Α	C
ATOM	1502	CB	ALA	213	52. 193	67.548	17. 224	1.00 14.16	Ā	Ċ
ATOM	1504	C	ALA	213	50. 429	66. 935	15. 526	1.00 15.57	A	Č
	1504	Ŏ	ALA	213	50. 857	67.862	14. 833	1.00 13.25	Ä	ŏ
ATOM			LEU	214	49. 448	66. 132	15. 129	1.00 14.75	Ä	Ň
ATOM	1506	N				66. 339	13. 123	1.00 14.10	A	Č
ATOM	1507	CA	LEU	214	48. 734			1.00 16.03	A	Č
ATOM	1508	CB	LEU	214	49. 353	65.517	12. 735			
ATOM	1509	CG	LEU	214	49. 482	63.999	12.823	1.00 17.01	A	C
ATOM	1510		LEU	214	48. 135	63. 342	12.628	1.00 18.97	A	C
ATOM	1511		LEU	214	50. 434	63. 535	11.742	1.00 16.98	A	Č
ATOM	1512	С	LEU	214	47. 273	65.963	14.124	1.00 16.65	A	C
ATOM	1513	0	LEU	214	46. 966	64.933	14.728	1.00 18.12	A	0
ATOM	1514	N	TRP	215	46. 366	66.811	13.666	1.00 16.16	Ą	Ŋ
ATOM	1515	CA	TRP	215	44. 959	66.590	13.907	1.00 14.69	A	C
ATOM	1516	CB	TRP	215	44. 471	67.663	14.863	1.00 15.49	A	C
ATOM	1517	CG	TRP	215	45. 230	67.669	16.145	1.00 17.52	Α	С
ATOM	1518		TRP	215	46. 482	68. 325	16.403	1.00 17.74	A	C
111 Out		720				-				

					5.1	0 4	0.0			(Continued)
					FI	G. 4	- 3 2			
ATOM	1519	CE2	TRP	215	46.852	68.008	17. 729	1.00 17.50	Α	C
ATOM	1520	CE3		215	47. 325	69. 149	15.643	1.00 18.21	A	C
ATOM	1521	CD1		215	44. 904	67.004	17. 289	1.00 15.79	A	Ç
ATOM	1522	NE 1		215	45. 873	67. 202	18. 243	1.00 17.35	A	N
ATOM	1523	CZ2		215	48. 033	68. 485	18.318	1.00 18.06	A	C
ATOM	1524	CZ3		215	48. 505	69. 625	16. 228	1.00 18.96	A	C
ATOM	1525	CH2		215	48. 844	69. 289	17. 555	1.00 18.21	A	C C
ATOM	1526		TRP	215	44. 110 43. 869	66.605	12. 661 12. 090	1.00 15.55 1.00 16.18	A A	0
ATOM	1527		TRP	215	43. 646	67. 668 65. 430	12. 244	1.00 15.15	A	N N
ATOM	1528		TRP TRP	216 216	42. 793	65. 330	11.069	1.00 16.40	A	Ċ
ATOM	1529 1530		TRP	216	42. 494	63.873	10. 739	1.00 16.43	Ä	č
ATOM ATOM	1531		TRP	216	43. 549	63. 114	10. 002	1.00 17.38	Ā	Č
ATOM	1532	CD2		216	43. 823	63. 169	8. 599	1.00 17.01	Α	C
ATOM	1533	CE2		216	44. 794	62. 176	8. 320	1.00 17.25	Α	C
ATOM	1534	CE3		216	43. 340	63.954	7.549	1.00 17.09		C
ATOM	1535	CD1		216	44.352	62.125	10.508	1.00 18.55	Α	C
ATOM	1536	NE1		216	45.098	61.553	9. 501	1.00 18.07	A	N
ATOM	1537	CZ2	TRP	216	45. 286	61.951	7.036	1.00 15.24	A	C
ATOM	1538	CZ3		216	43.829	63.729	6. 270	1.00 17.06	A	C
ATOM	1539	CH2		216	44. 794	62.734	6.027	1.00 17.07	A	C
ATOM	1540	C	TRP	216	41.461	66.016	11.355	1.00 17.17	A	C
ATOM	1541	0	TRP	216	40.990	66.005	12.487	1.00 18.00	A	0
ATOM	1542	N	SER	217	40.847		10.334	1.00 18.39	A	N
ATOM	1543	CA	SER	217	39. 552	67. 240	10.523	1.00 19.62	A	C
ATOM	1544	CB	SER	217	39. 257	68. 225	9.392	1.00 20.31	A A	C 0
ATOM	1545	0G	SER	217	39. 234		8. 133	1.00 24.00 1.00 20.47	A	Č
ATOM	1546	C	SER	217	38. 528	66. 108 64. 994	10.550 10.110	1.00 20.47	A	Ö
ATOM	1547 1548	O N	SER PRO	217 218	38. 814 37. 326	66.369	11.074	1.00 20.82	A	N
ATOM ATOM	1549	CD	PRO	218	36. 827		11.598	1.00 20.28	A	Ċ
ATOM	1550	CA	PRO	218	36. 285		11.154	1.00 22.67	A	
ATOM	1551	CB	PRO	218	35. 033	66.148	11.462	1.00 21.68	A	C C
ATOM	1552	CG	PRO	218	35. 587	67. 223	12.353	1.00 21.12	Α	C
ATOM	1553	C	PRO	218	36. 123		9.950	1.00 23.46	Α	C
ATOM	1554	Ŏ	PRO	218	36.190		10.107	1.00 25.13	Α	0
ATOM	1555	Ň	ASN	219	35. 909	64.948	8.756	1.00 22.93	Α	N
ATOM	1556	CA	ASN	219	35.756	64.071	7.600	1.00 22.31	Α	C
ATOM	1557	CB	ASN	219	34. 704		6. 631	1.00 22.48	A	Ċ
ATOM	1558	CG	ASN	219	35. 172		5.903	1.00 24.12	A	C
ATOM	1559		ASN	219	36. 373		5. 760	1.00 26.01	A	0
ATOM	1560		ASN	219	34. 230		5. 411	1.00 26.27	A	N
ATOM	1561	C	ASN	219	37. 090		6.871	1.00 21.20	A	C
ATOM	1562	0	ASN	219	37. 115		5. 760	1.00 20.94	A	0 N
ATOM	1563		GLY	220	38. 184		7. 499	1.00 18.33	A	N C
ATOM	1564		GLY	220	39. 512		6. 941	1.00 17.97 1.00 18.92	A A	C C
ATOM	1565		GLY	220	40.035		5. 853 5. 375	1.00 18.92	A	0
ATOM	1566		GLY	220 221	41.157 39.242		5. 447	1.00 20.28	A	N N
ATOM	1567	N	THR	441	JJ. 444	00.500	U: 771	1.00 11.01	21	•1

				E I C	4 00			(Conti	inued)
			224	FIG.		1 00 15 90	٨	C	
ATOM	1568	CA THR	221	39. 654 66. 93		1.00 15.80 1.00 15.67	A A	C C	
ATOM	1569	CB THR	221	38. 540 67. 94		1.00 15.01	A	0	
ATOM	1570	OG1 THR	221	37.410 67.20		1.00 10.41	A	C	
ATOM	1571	CG2 THR	221	39. 019 69. 00 40. 903 67. 6		1.00 12.30	A	č	
ATOM	1572	C THR	221	40.903 67.6° 41.884 67.7°		1.00 16.98	A	ŏ	
ATOM	1573	O THR	$\begin{array}{c} 221 \\ 222 \end{array}$	40. 864 68. 23		1.00 15.92	A	N	
ATOM	1574	N PHE CA PHE	222	41. 999 69. 0		1.00 15.88	Ä	Ċ	
ATOM	1575		222	41.508 70.2		1.00 15.20	A	Č	
ATOM	1576	CB PHE	222	40. 939 71. 30		1.00 14.35	A	č	
ATOM ATOM	1577 1578	CD1 PHE	222	39. 569 71. 5		1.00 11.89	A	Č	
ATOM	1579	CD1 THE	222	41. 782 72. 0		1.00 14.45	Ä	Č	
ATOM	1580	CE1 PHE	222	39.046 72.5		1.00 13.50	Ā	Č	
ATOM	1581	CE2 PHE	222	41. 269 73. 1		1.00 12.61	Ā	C	
ATOM	1582	CZ PHE	222	39. 897 73. 3		1.00 15.23	A	C	
ATOM	1583	C PHE	222	42.907 68.2		1.00 16.13	Α	С	
ATOM	1584	0 PHE	222	42.467 67.3		1.00 16.82	Α	0	
ATOM	1585	N LEU	223	44. 187 68. 5		1.00 15.93	Α	N	
ATOM	1586	CA LEU	223	45.159 67.9		1.00 14.81	Α	C	
ATOM	1587	CB LEU	223	46. 199 67. 1		1.00 14.64	Α	C	
ATOM	1588	CG LEU	223	47.306 66.6		1.00 14.94	Α	C	
ATOM	1589	CD1 LEU	223	46.696 65.7	73 9.687	1.00 11.99	Α	C	
ATOM	1590	CD2 LEU	223	48. 338 65. 8		1.00 11.50	Α	C	
ATOM	1591	C LEU	223	45. 848 69. 1		1.00 16.80	A	С	
ATOM	1592	0 LEU	223	46.398 70.0		1.00 16.53	A	0	
ATOM	1593	N ALA	224	45. 790 69. 2		1.00 17.34	A	N	
ATOM	1594	CA ALA	224	46. 420 70. 3		1.00 18.47	A	Č	
ATOM	1595	CB ALA	224	45. 422 70. 9		1.00 17.47	A	C	
ATOM	1596	C ALA	224	47. 596 69. 7		1.00 18.77	A	C	
ATOM	1597	O ALA	224	47. 587 68. 5		1.00 19.22	A	0	
ATOM	1598	N TYR	225	48.614 70.5		1.00 17.68	A	N	
ATOM	1599	CA TYR	225	49.764 70.0		1.00 17.56	A	C	
ATOM	1600	CB TYR	225	50.726 69.3		1.00 16.48	Ą	C C	
ATOM	1601	CG TYR	225	51. 273 70. 1		1.00 15.05	A	C	
ATOM	1602	CD1 TYR	225	50.551 70.2		1.00 13.44	A		
ATOM	1603	CE1 TYR	225	51.050 70.9		1.00 9.19	A	C	
ATOM	1604	CD2 TYR	225	52.514 70.7		1.00 14.42	A	C C C	
ATOM	1605	CE2 TYR	225	53.025 71.4		1.00 14.09	A A	C	
ATOM	1606	CZ TYR OH TYR	225 225	52. 286 71. 5 52. 802 72. 2		1.00 14.11 1.00 14.49	A	0	
MOTA	1607	C TYR	225	50. 514 71. 1		1.00 14.45	A	C	
MOTA	1608	0 TYR	225	50. 326 72. 3		1.00 17.79	A	0	
ATOM ATOM	1609 1610	N ALA	226	51.358 70.7		1.00 13.31	A	N	
ATOM	1611	CA ALA	226	52. 164 71. 7		1.00 17.74	A	Ċ	
ATOM	1612	CB ALA	226	52.060 71.4		1.00 18.89	A	C C	
ATOM	1613	C ALA	226	53.601 71.5		1.00 17.39	Ä	č	
ATOM	1614	O ALA	226	53. 966 70. 5		1.00 16.05	A	ŏ	
ATOM	1615	N GLN	227	54.412 72.6		1.00 17.45	A	Ň	
ATOM	1616	CA GLN	227	55.816 72.5		1.00 16.64	Ā	C	
				· · · · ·					

(Continued)

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FIG. 4-34 1.00 15.62 A 73.423 13. 331 56.096 CB GLN 227 ATOM 1617 1.00 16.35 A C 73.246 12.799 57.514 227 CG GLN ATOM 1618 C 1.00 14.31 A 74.191 11.666 57.847 CD GLN 227 ATOM 1619 1.00 18.11 A 0 75.408 11.851 57.877 GLN 227 1620 0E1 ATOM 73.639 1.00 12.45 A N 10.486 58, 101 GLN 227 **ATOM** 1621 NE2 1.00 16.27 A C 73.073 15.723 56.615 227 ATOM 1622 C GLN 1.00 16.33 0 16.225 56.346 74.159 1623 GLN 227 **ATOM** 0 N 16.158 1.00 17.36 A 72.301 57.601 1624 N PHE 228 ATOM 1.00 16.81 A C 17.287 72.717 58.414 1625 PHE 228 ATOM CA C 1.00 14.62 A 58.327 71.686 18.412 1626 CB PHE 228 **ATOM** C 1.00 14.48 A 56.919 71.295 18.758 CG PHE 228 1627 **ATOM** Č 70.196 1.00 14.37 56.317 18.141 Α CD1 PHE 228 **ATOM** 1628 C 72.03619.674 1.00 12.73 A 56.183 1629 CD2 PHE 228 **ATOM** C 69.840 18.430 1.00 13.56 Α 55.007 1630 CE1 PHE 228 **ATOM** C 71.691 19.971 1.00 14.73 A 54.870 1631 CE2 PHE 228 **ATOM** C 1.00 15.31 Α 54.279 70.588 19.348 1632 CZPHE 228 ATOM C 1.00 18.12 59.848 72.922 16.859 Α PHE 228 1633 C **ATOM** 1.00 17.47 0 60.410 72.121 16.112 Α PHE 228 1634 0 ATOM N 60.413 74.027 17.335 1.00 20.00 A ASN 229 1635 N ATOM 1.00 20.87 C 17.042 A 61.779 74.435 ASN 229 1636 CA ATOM C 1.00 21.57 75.857 16.474 A 61.767 ASN 229 1637 CB ATOM C 1.00 24.35 76.257 15.870 A 63.086 ASN 229 1638 CG **ATOM** 0 1.00 26.00 A 16.289 75.774 OD1 ASN 229 64.141 1639 ATOM N 1.00 25.62 A 63.025 77.153 14.887 ASN 229 1640 ND2 ATOM C 18.362 1.00 21.39 A 62.540 74.421 ASN 229 C ATOM 1641 62. 232 63. 516 0 75.200 19.269 1.00 21.52 A ASN 229 1642 0 ATOM 1.00 20.96 N Α 73.530 18.481 **ASP** 230 **ATOM** 1643 N C 19.706 1.00 22.78 64.300 73.444 A **ATOM** 1644 CA ASP 230 C 1.00 22.69 72.026 20.268 A 230 64.275 ATOM 1645 CB ASP C 1.00 22.37 71.551 20.580 A 1646 CG **ASP** 230 62.880 ATOM 0 1.00 21.57 21.689 A 1647 OD1 ASP 230 62.681 71.015 ATOM 0 61.993 71.705 19.713 1.00 21.82 A OD2 ASP 230 1648 **ATOM** Č 65.734 73.825 19.412 1.00 24.50 A **ASP** 230 1649 C **ATOM** 1.00 24.72 0 73.252 19.979 A ASP 230 66.663 ATOM 1650 0 N 1.00 25.87 A 231 65.904 74.803 18.527 THR ATOM 1651 N C 75.245 18.122 1.00 26.22 A 67.228 THR 231 **ATOM** 1652 CA C 17.109 1.00 27.87 Α 231 67.149 76.406 1653 CB THR ATOM 0 1.00 28.62 A 231 66.540 75.947 15.893 0G1 THR 1654 ATOM C 16.813 1.00 26.63 A 231 68.545 76.947 1655 ATOM CG2 THR C 75.688 19.280 1.00 26.77 A 68.099 231 C THR 1656 **ATOM** 19.375 0 1.00 27.34 69.254 75.277 A 0 231 THR 1657 **ATOM** 1.00 25.50 N 67.550 76.519 20.163 A 232 N ATOM 1658 GLU C 77.020 21.285 1.00 24.52 Α 232 68.329 1659 CA **GLU** ATOM C 78.526 21.397 1.00 28.36 Α 232 68.154 CB GLU 1660 **ATOM** C 79.281 20.171 1.00 34.72 A **GLU** 232 68.615 CG **ATOM** 1661 80.780 20.338 1.00 40.02 A 232 68.483 1662 CD **GLU ATOM** 19.363 1.00 44.21 Α 0 1663 0E1 GLU 23268.767 81.509 ATOM 1.00 42.26 0 81.232 21.444 Α OE2 GLU 23268.100 1664 **ATOM** C 1.00 22.97 232 76.377 22.627

SUBSTITUTE SHEET (RULE 26)

68.020

GLU

1665

ATOM

C

ATOM 1666 O GLU 232 68.331 76.942 23.679 1.00 20.81 A O ATOM 1667 VAL 233 67.416 75.194 22.596 1.00 20.32 A N ATOM 1668 CA VAL 233 67.416 75.194 22.596 1.00 20.32 A N ATOM 1668 CA VAL 233 65.525 72.912 74.997 23.832 1.00 17.88 A C ATOM 1670 CCI VAL 233 65.522 72.925 24.957 1.00 14.00 A C ATOM 1671 CC2 VAL 233 66.678 74.478 23.160 1.00 16.73 A C ATOM 1671 CC2 VAL 233 66.678 74.478 23.160 1.00 16.73 A C ATOM 1673 O VAL 233 68.94 72.728 23.606 1.00 16.00 A C ATOM 1673 O VAL 233 68.94 72.728 23.606 1.00 16.01 6.00 A C ATOM 1674 N PRO 234 68.788 73.927 25.504 1.00 14.51 A N ATOM 1674 CD PRO 234 68.313 74.907 26.494 1.00 14.51 A N ATOM 1676 CA PRO 234 68.313 74.907 26.494 1.00 14.51 A N ATOM 1676 CA PRO 234 69.914 73.162 26.040 1.00 13.93 A C ATOM 1676 CA PRO 234 69.914 73.162 26.040 1.00 13.93 A C ATOM 1678 CC PRO 234 69.914 73.162 26.040 1.00 13.93 A C ATOM 1678 CC PRO 234 68.387 71.200 26.041 1.00 13.93 A C ATOM 1678 CC PRO 234 68.487 71.200 27.00 17.30 17.30 A C ATOM 1678 CC PRO 234 68.487 71.200 27.00 17.30 17.32 A C ATOM 1678 CC PRO 234 68.487 71.200 27.00 17.30 17.30 A C ATOM 1679 C PRO 234 68.487 71.200 27.00 17.30 17.30 A C ATOM 1679 C PRO 234 68.487 71.200 27.00 17.30 17.30 A C ATOM 1688 CC PRO 234 68.487 71.200 27.00 17.30 17.30 A C ATOM 1688 CD PRO 234 68.487 71.200 27.00 17.30 17.30 A C ATOM 1688 CB LEU 235 70.16 70.887 25.900 1.00 16.20 A C ATOM 1680 N EU 235 70.16 70.887 25.901 1.00 16.20 A C ATOM 1680 N EU 235 70.16 70.887 25.900 1.00 16.20 A C ATOM 1680 CB LEU 235 71.506 68.912 24.718 1.00 11.30 1.30 A C ATOM 1680 CB LEU 235 70.600 68.743 27.71 1.00 11.30 1.30 A C ATOM 1689 N ILE 236 70.896 68.743 27.118 1.00 17.26 A C ATOM 1689 N ILE 236 70.446 67.696 27.472 1.00 11.90 A C ATOM 1689 N ILE 236 70.446 67.696 27.472 1.00 11.90 A C ATOM 1690 CA ILE 236 69.866 65.298 30.448 1.00 11.26 A C ATOM 1690 CA ILE 236 60.466 68.596 28.491 1.00 18.00 8.40 C ATOM 1690 CB ILE 236 70.866 66.899 28.644 1.00 12.68 A C ATOM 1690 CB ILE 236 70.866 66.899 28.644 1.00 12.68 A C ATOM 1690 CB ILE 236 70.866 66.899 28.668 1.0						ר ז	C 1.	. 25			(Continued)
ATOM 1667 N VAL 233 67.416 75.194 22.596 1.00 20.32 A N C ATOM 1668 CA VAL 233 67.091 74.499 23.832 1.00 17.88 A C ATOM 1669 CB VAL 233 65.585 73.618 23.648 1.00 17.88 A C ATOM 1670 CG1 VAL 233 65.585 73.618 23.648 1.00 17.88 A C ATOM 1671 CG2 VAL 233 65.522 72.925 24.957 1.00 14.00 A C ATOM 1671 CG2 VAL 233 68.694 72.728 23.606 1.00 16.73 A C ATOM 1672 C VAL 233 68.694 72.728 23.606 1.00 16.73 A C ATOM 1673 O VAL 233 68.694 72.728 23.606 1.00 16.94 A O ATOM 1673 O VAL 233 68.694 72.728 23.606 1.00 15.94 A O ATOM 1674 N PRO 234 68.788 73.927 25.504 1.00 14.51 A N ATOM 1676 CA PRO 234 68.313 74.907 26.494 1.00 14.51 A N ATOM 1676 CA PRO 234 69.914 73.162 26.040 1.00 13.03 A C ATOM 1676 CA PRO 234 69.914 73.162 26.040 1.00 13.93 A C ATOM 1677 CB PRO 234 69.643 71.663 25.987 1.00 16.20 A C ATOM 1679 C PRO 234 69.437 1.603 25.987 1.00 16.20 A C ATOM 1680 O PRO 234 68.487 71.220 25.041 1.00 15.73 A O ATOM 1680 C PRO 234 68.487 71.220 25.041 1.00 15.73 A O ATOM 1680 C PRO 234 68.487 71.220 25.041 1.00 16.20 A C ATOM 1680 C PRO 234 68.487 71.220 25.041 1.00 16.20 A C ATOM 1680 C PRO 234 68.487 71.220 25.041 1.00 16.20 A C ATOM 1680 C PRO 235 70.016 70.887 25.900 1.00 16.28 A N ATOM 1680 C PRO 235 71.505 68.912 24.718 1.00 16.29 A C ATOM 1680 C LEU 235 71.505 68.912 24.718 1.00 18.54 A C ATOM 1688 C LEU 235 71.505 68.912 24.718 1.00 18.54 A C ATOM 1688 C LEU 235 71.505 68.912 24.718 1.00 18.54 A C ATOM 1688 C LEU 235 70.602 69.946 68.790 22.768 1.00 16.91 A C ATOM 1688 C LEU 235 70.990 68.743 25.828 1.00 19.17 A C ATOM 1689 N ILE 236 69.946 68.890 22.768 1.00 16.91 A C ATOM 1689 N ILE 236 70.586 68.942 24.718 1.00 12.90 A C ATOM 1689 C LEU 235 70.990 68.743 27.718 1.00 12.90 A C ATOM 1693 C LEU 235 70.990 68.743 27.718 1.00 12.93 A C ATOM 1693 C LEU 235 70.990 68.743 27.718 1.00 12.93 A C ATOM 1699 C LEU 235 70.990 68.743 27.718 1.00 10.90 12.84 A C ATOM 1699 C LEU 235 70.866 68.249 28.860 1.00 19.17 A C ATOM 1699 C LEU 237 73.463 64.840 29.991 1.00 13.45 A C ATOM 1699 C LEU 237 73.463 64.80 29.992 8.719 1.00 13.45 A C	1 mc 1 1	1000		71 11	000				1 00 90 91	A	0
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ATOM 1703 OE2 GLU 237 76. 928 66. 324 26. 408 1. 00 26. 23 A O ATOM 1704 C GLU 237 73. 744 63. 427 29. 191 1. 00 13. 41 A C ATOM 1705 O GLU 237 73. 895 63. 752 30. 363 1. 00 14. 43 A O ATOM 1706 N TYR 238 73. 801 62. 169 28. 781 1. 00 12. 83 A N ATOM 1707 CA TYR 238 74. 052 61. 093 29. 721 1. 00 14. 06 A C ATOM 1708 CB TYR 238 72. 810 60. 840 30. 595 1. 00 12. 42 A C ATOM 1709 CG TYR 238 71. 566 60. 419 29. 856 1. 00 11. 79 A C ATOM 1710 CD1 TYR 238 71. 451 59. 139 29. 317 1. 00 16. 12 A C ATOM 1711 CE1 TYR 238 70. 292 58. 739 28. 635 1. 00 17. 09 A C ATOM 1712 CD2 TYR 238 70. 496 61. 295 29. 701 1. 00 12. 13 A C	ATOM	1701	CD	GLU							_
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ATOM 1712 CD2 TYR 238 70.496 61.295 29.701 1.00 12.13 A C											Ċ
114 4 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1											С
1110	ATOM				238	69. 336	60.913	29.020	1.00 12.94	A	С
ATOM 1714 CZ TYR 238 69. 243 59. 634 28. 487 1. 00 15. 48 A C						69. 243	59. 634	28. 487	1.00 15.48	A	С

				F.I.C. 4 - 2.6	((Continued)
				FIG. 4-36		
ATOM	1715	OH TYR	238	68. 127 59. 257 27. 775 1. 00 15. 96	_	0
ATOM	1716	C TYR	238	74. 445 59. 847 28. 954 1. 00 15. 25		C
ATOM	1717	0 TYR	238	12000	A	0 N
MOTA	1718	N SER	239	10122	A	N
ATOM	1719	CA SER	239	10.000	A	C
ATOM	1720	CB SER	239	10.000	A ^	C 0
ATOM	1721	OG SER	239		A ^	C
ATOM	1722	C SER	239	12,002	A A	Ö
ATOM	1723	0 SER	239		A	N
ATOM	1724	N PHE	240		A	Ċ
ATOM	1725	CA PHE CB PHE	240 240		A	č
ATOM	1726 1727	CB PHE CG PHE	240		A	č
ATOM ATOM	1728	CD1 PHE	240		A	Č
ATOM	1729	CD2 PHE	240		A	С
ATOM	1730	CE1 PHE	240		Α	C
ATOM	1731	CE2 PHE	240		A	С
ATOM	1732	CZ PHE	240	69.954 51.878 26.888 1.00 10.46	A	C
ATOM	1733	C PHE	240		A	С
ATOM	1734	0 PHE	240	1.4.1.	A	0
ATOM	1735	N TYR	241	***	A	N
ATOM	1736	CA TYR	241		A	C
ATOM	1737	CB TYR	241		A	C
ATOM	1738	CG TYR	241		A	C
ATOM	1739	CD1 TYR	241		A	C C
ATOM	1740	CE1 TYR	241	· · · · · · · · · · · · · · · · · · ·	A ^	C
ATOM	1741	CD2 TYR	241	, , , , , , , , , , , , , , , , , , , 	A A	C
ATOM	1742	CE2 TYR	241		A	Č
ATOM	1743	CZ TYR	241 241		A	0
ATOM	1744	OH TYR C TYR	241		A	Č
ATOM ATOM	1745 1746	0 TYR	241		Ä	Ŏ
ATOM	1747	N SER	242		Ä	N
ATOM	1748	CA SER	242		A	C
ATOM	1749	CB SER	242		Α	С
ATOM	1750	OG SER	242		Α	0
ATOM	1751	C SER	242		A	C
ATOM	1752	0 SER	242	75. 219 47. 625 27. 303 1. 00 19. 13	A	0
ATOM	1753	N ASP	243	· · · · · · · · · · · · · · · · · · ·	A	N
ATOM	1754	CA ASP	243		A	Č
ATOM	1755	CB ASP	243	******	A	C
ATOM	1756	CG ASP	243		Ä	C
ATOM	1757	OD1 ASP	243		A	0
ATOM	1758	OD2 ASP	243		A	0
ATOM	1759	C ASP	243		A	C
ATOM	1760	O ASP	243	111200	A	O N
ATOM	1761	N GLU	244		A A	C
ATOM	1762		244	100 112	A	C
ATOM	1763	CB GLU	244	78. 534 42. 984 27. 605 1. 00 23. 73	41	U

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										(Continued)
					FΙ	G. 4	- 37			(Continueu)
ATOM	1764	CG	GLU	244	79.940	42. 547	27. 995	1.00 29.35	Α	С
ATOM	1765	CD	GLU	244	79.967	41.177	28.667	1.00 29.80	Ā	C
ATOM	1766		GLU	244	81.079	40.680	28.958	1.00 29.53	Α	0
ATOM	1767	0E2	GLU	244	78. 877	40.601	28.903	1.00 29.32	Α	0
ATOM	1768	C	GLU	244	79. 374	44. 476	25. 754	1.00 22.28	Α	C
ATOM	1769	0	GLU	244	80. 533	44.854	25.913	1.00 21.94	Α	0
ATOM	1770	N	SER	245	78. 888	44. 159	24.561	1.00 21.62	Α	N
ATOM	1771	CA	SER	245	79. 724	44. 205	23. 370	1.00 19.92	Α	C
ATOM	1772	CB	SER	245	79.080	43. 402	22. 244	1.00 19.31	A	C
ATOM	1773	0G	SER	245	77. 949	44.068	21.723	1.00 17.93	A	0
ATOM	1774	C	SER	245	80.044	45. 605	22. 861	1.00 19.58	A	C
ATOM	1775	0	SER	245	80. 874	45. 762	21.971	1.00 21.35	A	0
ATOM	1776	N	LEU	246	79. 392	46. 628	23. 397	1.00 18.69	A	N
ATOM	1777	CA	LEU	246	79.694	47. 983	22.943	1.00 18.41	A	C
ATOM ATOM	1778 1779	CB CG	LEU LEU	246	78. 522	48. 926	23. 229	1.00 18.20	A	C
ATOM	1780	CD1		$\begin{array}{c} 246 \\ 246 \end{array}$	78. 659 78. 736	50. 368 50. 388	22. 728 21. 214	1.00 17.99 1.00 16.83	A	C
ATOM	1781	CD2		246	77. 458	51. 181	23. 192	1.00 10.83	A A	C C
ATOM	1782	C	LEU	246	80. 943	48. 463	23. 679	1.00 13.38	A	C
ATOM	1783	ŏ	LEU	246	80. 921	48. 662	24. 895	1.00 16.12	A	0
ATOM	1784	Ň	GLN	247	82. 034	48. 635	22. 940	1.00 17.84	A	N
ATOM	1785	ĊA	GLN	247	83. 295	49.073	23. 532	1.00 17.30	Ä	Ĉ
ATOM	1786	CB	GLN	247	84. 400	49.038	22. 480	1.00 15.11	A	č
ATOM	1787	CG	GLN	247	85.791	49. 234	23. 045	1.00 17.62	Ä	Č
ATOM	1788	CD	GLN	247	86.875	48.770	22.090	1.00 18.47	Ā	Č
ATOM	1789	0E1		247	86.829	49.065	20.899	1.00 20.53	Α	0
ATOM	1790	NE2		247	87.862	48.049	22.611	1.00 17.76	Α	N
ATOM	1791	C	GLN	247	83. 224	50.461	24. 170	1.00 17.66	Α	C
ATOM	1792		GLN	247	83.640	50.648	25. 313	1.00 17.56	Α	0
ATOM	1793	N ~	TYR	248	82. 710	51.436	23.430	1.00 18.50	Α	N
ATOM	1794	CA	TYR	248	82. 592	52. 794	23.954	1.00 19.00	Α	С
ATOM	1795	CB	TYR	248	83. 177	53. 822	22.972	1.00 17.39	A	C
ATOM	1796	CG	TYR	248	84. 684	53.820	22.860	1.00 16.80	A	C
ATOM	1797		TYR	248	85. 353	52.812	22.172	1.00 17.20	A	C
ATOM	1798			248	86. 742	52.814	22.058	1.00 17.58	A	C
ATOM ATOM	1799 1800	CD2 CE2		248	85. 444	54. 838	23. 437	1.00 17.77	A	C
ATOM	1801		TYR	248	86. 839	54.851	23. 333	1.00 17.22	A	C
ATOM	1802		TYR	248 248	87. 479	53.836	22.647	1.00 18.42	A	C
ATOM	1802		TYR	248	88. 854 81. 130	53. 809 53. 134	22. 595 24. 212	1.00 19.27 1.00 18.87	A	0
ATOM	1804		TYR	248	80. 288	53. 134	23. 323	1.00 18.87	A A	C 0
ATOM	1805		PRO	249	80. 804	53. 549	25. 440	1.00 13.13	A	N N
ATOM	1806		PRO	249	81.610	53. 595	26.668	1.00 18.20	A	C
ATOM	1807		PRO	249	79.411	53. 886	25.716	1.00 18.83	A	Č
ATOM	1808		PRO	249	79. 424	54. 222	27. 206	1.00 19.46	A	Č
ATOM	1809		PRO	249	80. 857	54. 582	27. 481	1.00 17.63	A	Č .
ATOM	1810		PRO	249	78. 937	55.042	24. 852	1.00 19.66	A	Č
ATOM	1811		PRO	249	79. 734	55.864	24. 413	1.00 20.92	Ä	ŏ
ATOM	1812		LYS	250	77.638	55.096	24.599	1.00 19.01	A	N

(Continued)

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					FI	G. 4	- 38			(Continuou)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1813 1814 1815 1816 1817 1818 1819 1820 1821 1822 1823 1824 1825 1826 1827 1828 1829	CB CCD CE NZ C O N CA CB OG1 CG2 C		250 250 250 250 250 250 250 251 251 251 251 251 252 252	77. 083 75. 933 76. 320 75. 197 75. 698 76. 966 76. 580 76. 130 76. 663 76. 171 77. 104 78. 280 76. 414 74. 832 74. 755 73. 779 72. 439	56. 158 55. 618 54. 428 54. 010 52. 938 53. 385 57. 320 57. 130 58. 524 59. 689 60. 887 60. 654 62. 137 60. 086 60. 572 59. 860 60. 205	23. 785 22. 936 22. 089 21. 152 20. 203 19. 546 24. 628 25. 758 24. 077 24. 786 24. 666 25. 441 25. 181 24. 205 23. 083 24. 977 24. 559	1. 00 19. 61 1. 00 23. 51 1. 00 28. 40 1. 00 30. 62 1. 00 32. 02 1. 00 17. 92 1. 00 17. 90 1. 00 14. 61 1. 00 15. 48 1. 00 13. 61 1. 00 15. 96 1. 00 17. 34 1. 00 17. 34 1. 00 15. 27 1. 00 16. 08	A A A A A A A	C C C C N C C C C C C C C C C C C C C C
ATOM ATOM ATOM	1830 1831 1832	CB CG1 CG2	VAL VAL VAL	252 252 252	71.405 69.987 71.595	59. 381 59. 832 57. 895	25. 355 25. 014 25. 050	1.00 16.76 1.00 16.29 1.00 13.65	A A A	C C C
ATOM ATOM ATOM ATOM	1833 1834 1835 1836	C O N CA	VAL VAL ARG ARG	252 252 253 253	72. 223 72. 443 71. 799 71. 568	61. 699 62. 212 62. 398 63. 831	23. 754 23. 842	1.00 18.46 1.00 19.01 1.00 19.18 1.00 18.54	A A A	O N
ATOM ATOM ATOM ATOM	1837 1838 1839 1840	CB CG CD NE	ARG ARG ARG ARG	253 253 253 253	72. 574 74. 014 75. 021 75. 797	64. 567 64. 439 65. 066 64. 044	22. 949 23. 457 22. 519 21. 822	1.00 19.46 1.00 24.49 1.00 29.04 1.00 35.89	A A A	C C C C
ATOM ATOM ATOM ATOM	1841 1842 1843 1844		ARG ARG ARG ARG	253 253 253 253	77. 013 77. 606 77. 633 70. 140	63. 647 64. 191 62. 699 64. 156	22. 185 23. 241 21. 497 23. 449	1.00 38.08 1.00 39.69 1.00 40.12 1.00 17.33	A A A	C N N C
ATOM ATOM ATOM ATOM	1845 1846 1847 1848	O N CA CB	ARG VAL VAL VAL	253 254 254 254	69. 690 69. 432 68. 033 67. 079	63. 802 64. 836 65. 196 64. 405	22. 362 24. 344 24. 125 25. 070	1.00 18.44 1.00 16.85 1.00 15.67 1.00 16.67	A A A	O N C C
ATOM ATOM ATOM ATOM	1849 1850 1851 1852		VAL VAL VAL VAL	254 254 254 254	65. 640 67. 308 67. 737 68. 122	66. 660 67. 186	24. 405 25. 450	1.00 16.79 1.00 17.24 1.00 14.62 1.00 15.12	A R R	0 C ·
ATOM ATOM ATOM ATOM ATOM	1853 1854 1855 1856 1857	N	PRO PRO PRO PRO PRO	255 255 255 255 255	67. 048 66. 677 66. 725 66. 064 66. 674	67. 340 66. 945 68. 749 69. 193 68. 265	23. 475 22. 105 23. 730 22. 431 21. 397	1.00 13.71 1.00 10.62 1.00 13.00 1.00 13.28 1.00 13.45	2 A 0 A 8 A	N C C C
ATOM ATOM ATOM ATOM	1858 1859 1860 1861	C 0	PRO PRO TYR TYR	255 255 256 256	65. 735 64. 663 66. 108 65. 304	68. 674 68. 086 69. 255 69. 194	24. 899 24. 772 26. 032 27. 242	1.00 13.86 1.00 13.58 1.00 13.63 1.00 11.65	6 A 8 A 8 A	C O N C

										(Continued)
					FΙ	G. 4	- 39			
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1862 1863 1864 1865 1866 1867 1868 1869 1870 1871 1872 1873 1874	CG CD1 CE1 CD2 CE2 CZ OH C O N CD	TYR TYR	256 256 256 256 256 256 256 256 256 257 257	65. 801 65. 044 64. 949 64. 296 64. 460 63. 799 63. 722 63. 060 65. 488 66. 559 64. 444 63. 174 64. 548	68. 006 67. 706 68. 646 68. 351 66. 460 66. 156 67. 105 66. 801 70. 492 70. 750 71. 325 71. 254 72. 593	28. 077 29. 351 30. 378 31. 571 29. 549 30. 735 31. 742 32. 909 28. 012 28. 553 28. 080 27. 334 28. 800	1. 00 10. 57 1. 00 10. 49 1. 00 9. 61 1. 00 7. 54 1. 00 9. 65 1. 00 11. 05 1. 00 10. 10 1. 00 10. 49 1. 00 12. 70 1. 00 15. 49 1. 00 12. 39 1. 00 13. 82 1. 00 11. 47	A A A A A A A A A A	C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM	1875 1876	CB	PRO PRO	257 257	63. 501 62. 405	73. 450 72. 464	28. 106 27. 866	1.00 12.01 1.00 12.87	A A	C C
ATOM ATOM ATOM ATOM	1877 1878 1879 1880	C O N	PRO PRO LYS LYS	257 257 257 258 258	64. 296 63. 174 65. 327 65. 155	72. 489 72. 210 72. 718 72. 671	30. 298 30. 723 31. 105 32. 546	1.00 12.85 1.00 15.59 1.00 11.64 1.00 11.10	A A A	C O N C
ATOM ATOM	1881 1882	CB CG	LYS LYS	258 258	66. 501 67. 034	72. 439 71. 012	33. 227 33. 031	1.00 12.96 1.00 14.20	A A	C C
ATOM ATOM	1883 1884 1885	CD CE NZ	LYS LYS LYS	258 258 258	68. 519 69. 042 68. 671	70. 906 69. 480 68. 536	33. 331 33. 136 34. 223	1.00 13.34 1.00 13.95 1.00 10.80	A A A	C C N
ATOM ATOM ATOM	1886 1887	C O	LYS LYS	258 258 258	64. 517 64. 368	73. 984 74. 921	33. 011 32. 224	1.00 10.30 1.00 12.44 1.00 11.13	A A	C O
ATOM ATOM	1888 1889	N CA	ALA ALA	259 259	64. 124 63. 484	74. 043 75. 236	34. 280 34. 844	1.00 13.33 1.00 14.81	A A	N C
ATOM ATOM	1890 1891	CB C	ALA ALA	259 259	63. 368 64. 167	75. 097 76. 555	36. 355 34. 508	1.00 16.40 1.00 15.14	A A	C C
ATOM ATOM	1892 1893	O N CA	ALA GLY GLY	259 260	65. 317 63. 448 63. 984	76. 787 77. 419 78. 720	34. 881 33. 802 33. 444	1.00 17.32 1.00 16.82 1.00 15.59	A A A	O N C
ATOM ATOM ATOM	1894 1895 1896	CA C	GLY GLY	260 260 260	64. 870 65. 379	78. 749 79. 812	32. 217 31. 852	1.00 15.78 1.00 17.65	A A	Č 0
ATOM ATOM ATOM	1897 1898 1899	N CA CB	ALA ALA ALA	261 261 261	65.072 65.906 66.524	77. 600 77. 554 76. 182	31.577 30.379 30.224	1.00 13.77 1.00 11.19 1.00 10.21	A A A	N C C
ATOM ATOM ATOM	1900 1901 1902	C O N	ALA ALA VAL	261 261 262	65. 093 63. 896 65. 747	77. 911 78. 160 77. 947	29. 137 29. 212 27. 987	1.00 10.04 1.00 8.71 1.00 11.73	A A A	C O N
ATOM ATOM ATOM	1903 1904 1905	CA CB CG1	VAL VAL VAL	262 262 262	65. 050 66. 035 65. 257	78. 284 78. 529 78. 796	26. 761 25. 594 24. 299	1.00 12.13 1.00 11.50 1.00 8.31	A A A	C C C
ATOM ATOM ATOM	1906 1907 1908	C 0	VAL VAL VAL	262 262 262	66. 939 64. 092 64. 471	79. 732 77. 167 76. 001	25. 920 26. 389 26. 341	1.00 5.79 1.00 13.92 1.00 16.73	A A A	C C O
ATOM ATOM	1909 1910	N CA	ASN ASN	263 263	62. 844 61. 816	77. 536 76. 585	26. 139 25. 773	1.00 13.49 1.00 13.67	A A	N C

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					FΙ	G. 4	- 40			,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	inued)	
ATOM	1011	СВ	ASN	263	60. 470	77. 038	26. 336	1.00 14.53	Α	С		
ATOM	1911		asn Asn	263	60. 222	76. 545	27.746	1.00 17.27	Ä	Č		
ATOM	1912 1913	0D1		263	59. 342	77. 058	28. 444	1.00 18.62	A	Õ		
ATOM	1913	ND2		263	60. 977	75. 534	28. 169	1.00 16.78	Α	N		
ATOM ATOM	1914		ASN	263	61.715	76.500	24. 265	1.00 14.45	Α	C		
ATOM	1916		ASN	263	62. 170	77. 395	23. 561	1.00 16.33	Α	0		
ATOM	1917		PRO	264	61, 119	75.418	23.743	1.00 14.86	Α	N		
ATOM	1918		PRO	264	60. 513	74. 254	24.412	1.00 15.86	Α	С		
ATOM	1919		PRO	264	60.986	75.301	22.294	1.00 15.41	Α	C		
ATOM	1920		PR0	264	60.591	73.844	22.106	1.00 14.97	Α	Ç		
ATOM	1921		PR0	264	59.721	73.607	23. 287	1.00 14.81	A	Ċ		
ATOM	1922		PR0	264	59.867	76.238	21.882	1.00 15.66	A	C		
ATOM	1923	0	PR0	264	58. 954	76.496	22.663	1.00 17.42	A	0		
ATOM	1924		THR	265	59. 942	76. 767	20.673	1.00 15.76	Ą	N		
ATOM	1925		THR	265	58. 895	77.648	20. 199	1.00 14.67	A	C		
ATOM	1926		THR	265	59. 458		19.341	1.00 15.37	A	C		
ATOM	1927	0G1		265	60. 162	78. 228	18. 223	1.00 15.98	A	0		
ATOM	1928	CG2		265	60. 402		20. 159	1.00 12.01	A	C C		
ATOM	1929	C	THR	265	58. 024		19.360	1.00 15.62 1.00 18.75	A A	Õ		
ATOM	1930	0	THR	265	58. 465	75. 683 77. 170	18. 932 19. 113	1.00 18.75	A	N		
ATOM	1931		VAL	266	56. 794 55. 872		18. 347	1.00 13.30	A	Č		
ATOM	1932	CA CB	VAL VAL	$\begin{array}{c} 266 \\ 266 \end{array}$	54. 856		19. 274	1.00 12.13	A	Č		
ATOM ATOM	1933 1934	CG1		266	54. 193	76. 766	20. 130	1.00 12.06	Ä	Č		
ATOM	1935	CG2		266	53. 821	74. 920	18. 466	1.00 10.69	A	č		
ATOM	1936	C	VAL	266	55. 115		17. 350	1.00 12.88	Ā	Ċ		
ATOM	1937	ŏ	VAL	266	54. 995		17.511	1.00 12.12	Α	0		
ATOM	1938	Ň	LYS	267	54.601		16.327	1.00 13.52	Α	N		
ATOM	1939	ĊA	LYS	267	53.817		15.262	1.00 13.08	Α	C		
ATOM	1940	CB	LYS	267	54. 692		14.050	1.00 13.64	, A	C		
ATOM	1941	CG	LYS	267	55. 642		14. 165	1.00 13.17	Α	C		
ATOM	1942	CD	LYS	267	56. 348		12.833	1.00 11.33	A	C		
ATOM	1943	CE	LYS	267	57. 313		12. 788	1.00 11.66	A	C		
ATOM	1944	NZ	LYS	267	58. 007	79.844	11.459	1.00 12.98	Ą	N		
ATOM	1945	C	LYS	267	52. 713	76.136	14.851	1.00 14.81	A	C		
ATOM	1946	0	LYS	267	52. 885		14. 930	1.00 14.91	A	0		
ATOM	1947	N	PHE	268				1.00 15.02	A			
ATOM	1948	CA	PHE	268	50. 471		13.975	1.00 14.84	A	C		
ATOM	1949	CB	PHE	268	49. 249		14. 842 14. 846	1.00 13.98 1.00 15.65	A A	C		
ATOM	1950	CG	PHE	268	48. 237 48. 4 67		15. 562	1.00 15.53	A	Č		
ATOM	1951 1952		PHE PHE	268 268	48. 461 47. 056		14. 115	1.00 18.05	A	Ç		
ATOM	1952		PHE	268	47. 537		15. 551	1.00 15.00	A	č		
ATOM ATOM	1954		PHE	268	46. 120		14. 101	1.00 17.28	A	č		
ATOM	1955	CEZ	PHE	268	46. 366		14. 821	1.00 14.54	A	Č		
ATOM	1956	C	PHE	268	50.117		12. 497	1.00 14.63	A	Č		
ATOM	1957	ŏ	PHE	268	50. 143		11.981	1.00 16.53	Ā	0		
MOTA	1958	Ň	PHE	269	49. 767		11.829	1.00 13.37	Α	N		
ATOM	1959	CA	PHE	269	49.417		10.413	1.00 12.73	Α	C		

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(Continued) FIG. 4-41 **ATOM** 1960 CB PHE 269 50.597 74.510 9.547 1.00 12.68 C ATOM 1961 CG PHE 269 51.875 75. 229 9.809 1.00 10.71 $_{\rm C}^{\rm C}$ 52.190 ATOM 1962 CD1 PHE 269 76.387 9.112 1.00 11.11 A ATOM 1963 CD2 PHE 269 52.758 74.759 10.770 C 1.00 11.04 A **ATOM** 1964 CE1 PHE 53.374 77.070 269 9.371 C 1.00 12.54 53. 940 54. 252 48. 270 ATOM 1965 CE2 PHE 269 75.430 11.039 Č 1.00 13.96 Α **ATOM** 1966 CZ PHE 76.591 269 10.339 1.00 13.89 C Α **ATOM** 1967 PHE 74.032 C 269 10.117 1.00 12.37 C Α ATOM 1968 0 47.937 73.157 PHE 269 10.910 1.00 14.50 0 47.699 **ATOM** 1969 N 74.193 VAL 270 8.938 1.00 13.63 A N **ATOM** 1970 CA VAL 270 46.626 73.334 8.485 1.00 15.44 C ATOM 1971 CB VAL 270 45.228 73.903 8.815 1.00 14.59 C ATOM 1972 44.153 CG1 VAL 270 72.900 8.383 1.00 12.94 C Α 1973 ATOM CG2 VAL 270 45.110 74.183 10.304 1.00 15.69 A C ATOM 1974 46.730 C VAL 270 73.198 6.975 1.00 16.91 A \mathbf{c} ATOM 1975 0 VAL 270 46.875 74.188 6.258 1.00 17.51 A 0 **ATOM** 1976 N VAL 271 46.681 71.966 6.494 1.00 17.37 A N 1977 46.726 ATOM CA 271 VAL 71.746 5.067 1.00 16.54 A C 1978 **ATOM** CB VAL 271 47.928 70.879 4.646 1.00 19.07 A C ATOM 1979 CG1 VAL 271 47.911 69.548 5.400 1.00 20.07 C A ATOM 1980 CG2 47.878 VAL 271 70.635 1.00 18.62 3.131 A C **ATOM** 1981 45. 456 C VAL 271 71.041 4.641 1.00 15.09 Α C 1982 1983 **ATOM** 0 VAL 44.912 271 70.226 5.383 1.00 13.46 A 0 ATOM N ASN 272 44.988 71.394 3.449 1.00 15.17 A N ATOM 1984 CA ASN 272 43.812 70.802 2.832 1.00 14.94 A C ATOM 1985 43. 231 CB ASN 272 71.767 1.797 1.00 13.83 Α C 1986 1987 **ATOM** 42.010 CG ASN 272 71.205 1.093 1.00 14.46 A C ATOM 0D1 ASN 41.822 272 69.989 1.007 1.00 16.67 A 0 41.175 ATOM 1988 ND2 272 ASN 72.090 0.581 1.00 15.74 A N 1989 1990 ATOM ATOM 272 C ASN 44.310 1.00 15.70 69.542 2.110 C 0 **ASN** 272 44.755 69.617 0.967 1.00 16.88 A 0 **ATOM** 1991 68.390 N 273 THR 44. 241 2.758 1.00 15.93 A N 1992 1993 **ATOM** CA 273 THR 44.717 67.169 2.124 1.00 18.97 C A ATOM 273 CB THR 44.570 65.936 3.052 1.00 19.44 C A ATOM 1994 0G1 273 43. 201 THR 65.794 3.471 1.00 19.69 Α 0 ATOM 1995 CG2 273 45.481 THR 66.083 4.266 1.00 19.20 C A **ATOM** 1996 C 273 44.009 THR 66.870 0.813 1.00 19.92 C A ATOM 1997 0 273 THR 44.550 66.154 -0.0281.00 21.20 0 Α ATOM 1998 N 42. 811 42. 032 274 67.424 ASP 0.634 1.00 20.50 N A 1999 **ATOM** CA **ASP** 274 67.193 -0.584 1.00 20.30 C A ATOM 2000 CB **ASP** 274 40.578 67.629 -0.3901.00 21.02 $_{\rm C}^{\rm C}$ A ATOM 2001 CG 274 ASP 39.705 66.529 0.178 1.00 23.48 A **ATOM** 2002 0D1 ASP 274 38. 543 66.823 0.527 1.00 26.38 0 A **ATOM** 2003 **OD2** ASP 274 40.168 65.375 0.275 1.00 23.88 0 A ATOM 2004 C **ASP** 274 67.870 42.573 1.00 19.89 -1.832C A ATOM 2005 0 **ASP** 274 42.131 67.556 -2.9321.00 22.08 0 A ATOM 2006 N SER 275 43.508 68.802 -1.6761.00 18.13 N A ATOM 2007 CA SER 275 44.073 69.490 -2.8341.00 18.83 C **ATOM** 2008 CB SER 275 44.284 70.969 C 1.00 19.37 -2.518

		(Continued)							
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2009 2010 2011 2012 2013 2014 2015 2016 2017 2018 2019	C S S O S S N I CA I CB I CCD	SER 2 SER 2 LEU 2	75 45. 197 75 45. 397 75 45. 883 76 45. 971 76 47. 241 76 47. 725 76 47. 991 76 48. 875 76 47. 360 76 48. 290	71. 121 68. 885 69. 226 67. 986 67. 348 66. 226 66. 641 65. 410 67. 622 66. 790 67. 137	-1. 444 -3. 314 -4. 394 -2. 516 -2. 846 -1. 849 -0. 392 0. 456 -0. 277 -4. 263 -4. 994	1. 00 24. 82 1. 00 19. 53 1. 00 19. 59 1. 00 19. 83 1. 00 20. 72 1. 00 19. 96 1. 00 20. 47 1. 00 21. 68 1. 00 18. 56 1. 00 22. 34 1. 00 24. 63	A A A A A A A A	0 C O N C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2020 2021 2022 2023 2024 2025 2026	CA S CB S CC S CC S CC S CC S CC S CC S	SER 2'	77 46. 434 77 46. 501 77 45. 456 77 44. 148 77 46. 305 77 46. 699 78 45. 698	65. 925 65. 325 64. 219 64. 756 66. 341 66. 104 67. 472	-4. 656 -5. 983 -6. 121 -6. 044 -7. 097 -8. 231 -6. 768	1.00 22.80 1.00 23.82 1.00 22.59 1.00 23.44 1.00 24.47 1.00 26.86 1.00 25.44	A A A A A	N C C O C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2027 2028 2029 2030 2031 2032 2033	CB S OG S O	SER 2' SER 2' SER 2' SER 2' VAL 2' VAL 2'	78 45. 431 78 44. 051 78 43. 831 78 46. 495 78 46. 603 79 47. 277 79 48. 327	68. 522 69. 121 70. 266 69. 630 70. 414 69. 692 70. 696	-7. 745 -7. 471 -8. 266 -7. 739 -8. 683 -6. 672 -6. 565	1.00 26.20 1.00 25.70 1.00 30.53 1.00 25.70 1.00 23.48 1.00 26.01 1.00 28.42	A A A A A	C C O C O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2034 2035 2036 2037 2038 2039 2040	CG1 V CG2 V C V O V N T	VAL 2' VAL 2' VAL 2' VAL 2' THR 2:	79 48. 073 79 49. 372 79 47. 148 79 49. 704 79 49. 834 80 50. 728 80 52. 092	71. 634 72. 211 72. 768 70. 043 68. 872 70. 801 70. 306	-5. 350 -4. 834 -5. 776 -6. 470 -6. 088 -6. 848 -6. 832	1.00 29.96 1.00 32.19 1.00 29.00 1.00 28.21 1.00 29.00 1.00 26.67 1.00 26.53	A A A A A A	C C C C O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2041 2042 2043 2044	CB 1 0G1 7 CG2 7 C 1 O 1 N A	THR 23 THR 23 THR 23	30 53. 023 30 52. 533 30 54. 422 30 52. 618 30 53. 184 31 52. 402	71. 217 71. 331 70. 645 70. 254 69. 255 71. 341 71. 474	-7. 645 -8. 986 -7. 674	1.00 27.22 1.00 29.98 1.00 26.85 1.00 26.01 1.00 27.33 1.00 25.17 1.00 23.78	A A A A A A	C O C C O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2048 2049 2050 2051 2052 2053 2054	CB A CG A OD1 A ND2 A C A O A	ASN 28 ASN 28 ASN 28	31 54. 190 31 54. 925 31 54. 603 31 55. 948 31 51. 818 31 51. 876	72. 250 72. 287 71. 576 73. 136 72. 211 73. 431 71. 460	-3. 388 -2. 071 -1. 116 -2. 056 -2. 506 -2. 362 -1. 982	1. 00 22. 28 1. 00 22. 87 1. 00 20. 83 1. 00 22. 18 1. 00 23. 12 1. 00 22. 47 1. 00 23. 33	A A A A A A	C C O N C O N
ATOM ATOM ATOM	2055 2056 2057	CA A	ALA 28 ALA 28 ALA 28	32 49. 763 32 48. 952	72. 018 70. 895 72. 912	-1. 166 -0. 547 -0. 071	1.00 23.40 1.00 23.19 1.00 24.45	A A A	C C C

					FI	G. 4 -	4 3			(Continued)
ATOM	2058	0	ALA	282	51.180	72.487	0.694	1.00 25.49	A	0
ATOM	2059		THR	283	49.817	74.140	0.024	1.00 24.70	Α	N
ATOM	2060		THR	283	50. 326	75.074	1.021	1.00 25.33	Α	C
ATOM	2061		THR	283	50. 209	76.540	0.539	1.00 27.36	Α	C
ATOM	2062		THR	283	48.834	76.874	0.353	1.00 29.84	A	0
ATOM	2063		THR	283	50.947	76.730	-0.785	1.00 30.06	A	C
ATOM	2064	C	THR	283	49.710	74.983	2.406	1.00 24.49	A	C
ATOM	2065		THR	283	48. 487	74.960	2.578	1.00 24.13	A	0 N
ATOM	2066	N	SER	284	50. 593	74. 941	3.396	1.00 23.17	A	N C
ATOM	2067	CA	SER	284	50. 200	74.872	4. 791	1.00 19.88	A	C C
ATOM	2068	CB	SER	284	51.317	74. 249	5.624	1.00 15.88	A	0
ATOM	2069	0G	SER	284	51.413	72.868	5.350	1.00 14.23 1.00 19.24	A A	C
ATOM	2070	C	SER	284	49.906	76. 275	5. 288 5. 253	1.00 19.24	A	0
ATOM	2071	0	SER	284	50.774	77.148	5. 745	1.00 17.36	A	N N
ATOM	2072	N CA	ILE	285	48. 674 48. 249	76.478 77.771	6. 242	1.00 16.16	A	C
ATOM	2073	CA	ILE	285 285	46. 754	78.003	5. 977	1.00 16.10	A	č
ATOM	2074	CB CG2	ILE ILE	285	46. 384	79.446	6.324	1.00 14.55	Ä	č
ATOM ATOM	2075 2076	CG2 CG1		285	46.434	77.691	4.513	1.00 14.89	Ä	C C
ATOM	2077		ILE	285	47. 230	78. 526	3. 528	1.00 15.03	A	Č
ATOM ATOM	2078	C	ILE	285	48. 496	77.848	7. 733	1.00 16.46	Ā	Ċ
ATOM	2079	ŏ	ILE	285	48. 116	76.963	8.489	1.00 18.69	Α	0
ATOM	2080	N	GLN	286	49. 130	78.923	8.159	1.00 16.66	Α	N
ATOM	2081	CA	GLN	286	49. 428	79.088	9.563	1.00 16.43	Α	C
ATOM	2082	CB	GLN	286	50. 778	79.776	9.717	1.00 16.31	Α	С
ATOM	2083	CG	GLN	286	51.184	80.070	11.135	1.00 17.85	A	C
ATOM	2084	CD	GLN	286	52.552	80.713	11.196	1.00 21.44	A	C
ATOM	2085	0E1	GLN	286	53.072	81.005	12.277	1.00 24.09	Ą	0
ATOM	2086	NE2	GLN	286	53. 149	80.939	10.028	1.00 19.13	A	N
ATOM	2087	C	GLN	286	48. 360	79. 885	10. 289	1.00 16.82	A	C
ATOM	2088	0	GLN	286	47. 794	80.844	9.754	1.00 17.23	A	0 N
ATOM	2089	N	ILE	287	48. 070	79.453	11.507	1.00 15.99	A	N C
ATOM	2090	CA	ILE	287	47.116	80. 137	12.355 12.894	1.00 15.11 1.00 14.14	A A	C
ATOM	2091	CB	ILE	287	46.036	79. 182 79. 916	12. 894	1.00 14.14	A	C
ATOM	2092		ILE ILE	287 287	45. 147 45. 206	78. 621	11.742	1.00 13.29	A	č
ATOM	2093 2094	CG1 CD1	ILE	287	44. 111	77. 675	12. 202	1.00 14.31	A	č
ATOM ATOM	2094	CDI	ILE	287	47. 991	80. 625	13. 506	1.00 15.35	Ä	č
ATOM	2096	Ö	ILE	287	48. 349	79, 860	14. 401	1.00 14.39	A	Ö
ATOM	2097	N	THR	288	48. 367	81.894	13, 452	1.00 15.01	Ā	N
ATOM	2098	CA	THR	288	49. 215	82. 465	14. 482	1.00 16.71	A	C
ATOM	2099	CB	THR	288	49.688	83. 874	14.093	1.00 17.36	Α	С
ATOM	2100	0G1	THR	288	48. 548	84.679	13.779	1.00 21.17	Α	0
ATOM	2101	CG2		288	50.621	83.813	12.881	1.00 17.64	Α	C
ATOM	2102		THR	288	48.510	82.553	15.818	1.00 16.02	Α	C
ATOM	2103		THR	288	47. 287	82.668	15.888	1.00 16.28	Α	0
ATOM	2104		ALA	289	49. 301	82.488	16.881	1.00 16.31	A	N
ATOM	2105		ALA	289	48. 787	82. 582	18. 232	1.00 16.67	A	C
ATOM	2106	CB	ALA	289	49. 887	82. 262	19. 207	1.00 18.89	A	С

				FIG. 4-44	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2108 2109 2110 2111 2112 2113 2114 2115 2116 2117 2118 2119 2120 2121 2122	C ALA O ALA N PRO CD PRO CA PRO CG PRO O PRO N ALA CA ALA CB ALA C ALA N SER CA SER	291 291 292 292	48. 280 84. 001 18. 467 1. 00 18. 05 A 48. 629 84. 927 17. 733 1. 00 19. 12 A 47. 436 84. 193 19. 487 1. 00 18. 60 A 46. 851 83. 189 20. 388 1. 00 18. 37 A 46. 906 85. 526 19. 783 1. 00 19. 04 A 45. 791 85. 234 20. 777 1. 00 17. 58 A 46. 306 84. 055 21. 499 1. 00 19. 78 A 47. 976 86. 447 20. 369 1. 00 20. 45 A 48. 866 85. 995 21. 092 1. 00 22. 14 A 47. 878 87. 735 20. 054 1. 00 19. 85 A 48. 829 88. 728 20. 543 1. 00 19. 27 A 48. 330 90. 132 20. 213 1. 00 17. 30 A 49. 101 88. 610 22. 041 1. 00 19. 66 A 50. 238 88. 791 22. 489 1. 00 21. 52 A 48. 074 88. 305 22. 825 1. 00 19. 16 A 48. 275 <	C O N C C C C C C O N C C C C O N C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2123 2124 2125 2126 2127 2128 2129 2130 2131 2132 2133 2134 2135 2136 2137	CB SER C SER O SER N MET CA MET CB MET CG MET C MET C MET O MET N LEU CA LEU CB LEU	292 292 292 293 293 293 293 293 293 293	46. 936 87. 983 24. 971 1. 00 19. 90 A 46. 259 86. 839 24. 487 1. 00 24. 94 A 49. 244 87. 055 24. 618 1. 00 20. 24 A 49. 686 86. 948 25. 760 1. 00 21. 86 A 49. 566 86. 214 23. 635 1. 00 20. 06 A 50. 504 85. 104 23. 818 1. 00 18. 78 A 49. 987 83. 830 23. 149 1. 00 17. 35 A 48. 795 83. 168 23. 797 1. 00 15. 90 A 49. 139 82. 503 25. 424 1. 00 15. 89 A 47. 655 82. 993 26. 296 1. 00 16. 41 A 51. 831 85. 487 23. 161 1. 00 20. 24 A 52. 912 85. 221 23. 693 1. 00 21. 12 A 51. 738 86. 116 21. 995 1. 00 20. 44 A 52. 918 86. 532 21. 255 1. 00 21. 31 A 52. 498 87. 104 19. 900 1. 00 21. 19 A	C O C O N C C C S C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2138 2139 2140 2141 2142 2143 2144 2145 2146 2147 2148 2150 2151 2152 2153 2154 2155	CG LEU CD1 LEU CD2 LEU C LEU O LEU N ILE CA ILE CG2 ILE CG1 ILE CG2 ILE CG1 ILE CG2 ILE CG1 IL	294 294 294 295 295 295 295 295 295 295 296 296 296 296 296	51. 850 86. 092 18. 944 1. 00 23. 63 A 51. 257 86. 820 17. 747 1. 00 22. 60 A 52. 889 85. 064 18. 493 1. 00 20. 94 A 53. 818 87. 533 21. 981 1. 00 22. 05 A 54. 953 87. 742 21. 564 1. 00 23. 39 A 53. 329 88. 156 23. 053 1. 00 21. 86 A 54. 149 89. 122 23. 792 1. 00 22. 24 A 53. 323 89. 938 24. 835 1. 00 24. 92 A 52. 084 90. 536 24. 196 1. 00 25. 08 A 52. 906 89. 034 25. 998 1. 00 25. 57 A 55. 271 88. 426 24. 565 1. 00 26. 45 A 55. 271 88. 426 24. 565 1. 00 23. 91 A 55. 154 87. 119 24. 749 1. 00 20. 65 A 56. 174 86. 401 25. 482 1. 00 1	C C O N C C

	٠			FIG. 4-45	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2170 2171 2172 2173 2174 2175 2176 2177 2178 2180 2181 2182 2183 2184 2185 2186 2187 2188 2189 2190 2191	CA ASP CB ASP CG ASP OD1 ASP OD2 ASP C ASP O ASP N HIS CA HIS CB HIS CCD HIS ND1 HIS CE1 HIS NE2 HIS C HIS CE1 TYR CA TYR CB TYR CCB T	297 297 297 297 297 298 298 298 298 298 299 299 299 299 299	56. 918 82. 694 25. 751 1. 00 16. 95 A 57. 960 82. 032 26. 650 1. 00 18. 00 A 59. 366 82. 378 26. 253 1. 00 18. 62 A 59. 553 82. 882 25. 128 1. 00 18. 23 A 60. 284 82. 134 27. 063 1. 00 21. 29 A 55. 553 82. 096 26. 041 1. 00 16. 02 A 54. 847 82. 537 26. 942 1. 00 16. 36 A 55. 190 81. 079 25. 279 1. 00 14. 79 A 53. 901 80. 449 25. 460 1. 00 16. 82 A 52. 846 81. 207 24. 661 1. 00 14. 81 A 53. 245 81. 448 23. 241 1. 00 15. 31 A 54. 127 82. 442 22. 876 1. 00 13. 01 A 54. 327 82. 392 21. 572 1. 00 14. 39 A 53. 608 81. 400 21. 076 1. 00 14. 38 A 53. 956 79. 008 24. 979 1. 00 17. 54 A 55. 066 <	
ATOM ATOM ATOM	2193 2194 2195	N CYS CA CYS CB CYS	301 301 301	48. 629 74. 290 23. 873 1. 00 17. 21 A 48. 288 73. 202 24. 782 1. 00 22. 20 A 48. 208 73. 722 26. 220 1. 00 22. 63 A	N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2196 2197 2198 2199 2200 2201 2202 2203	SG CYS C CYS O CYS N ASP CA ASP CB ASP CG ASP OD1 ASP	301 301 302 302 302 302 302 302	46. 943 74. 962 26. 503 1. 00 26. 56 A 47. 032 72. 399 24. 468 1. 00 23. 29 A 46. 690 71. 481 25. 210 1. 00 25. 66 A 46. 341 72. 731 23. 386 1. 00 23. 55 A 45. 148 71. 976 23. 015 1. 00 24. 19 A 43. 999 72. 223 23. 991 1. 00 26. 49 A 42. 789 71. 355 23. 680 1. 00 28. 68 A 42. 795 70. 170 24. 066 1. 00 30. 65 A	S C O C C C
ATOM	2204	OD2 ASP	302	41. 841 71. 844 23. 029 1. 00 30. 37 A	

(Continued)

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					FI	G. 4-	46			Conmidea
ATOM ATOM	2205 2206		ASP ASP	302 302	44. 658 44. 523	72. 292 73. 455	21.610 21.226	1.00 23.22 1.00 24.26	A A	C 0
ATOM	2207		/AL	303	44. 385	71. 237	20. 857 19. 493	1.00 21.65 1.00 20.79	A A	N C
ATOM	2208		/AL	303 303	43. 902 44. 926	71. 349 70. 803	18. 480	1.00 20.13	A	č
ATOM ATOM	2209 2210	CB V	VAL VAT	303	44. 420	71.028	17.051	1.00 20.34	Ä	C
ATOM	2211	CG2 V		303	46. 273	71.465	18.702	1.00 20.12	Α	C
ATOM	2212		VAL	303	42.657	70.494	19.417	1.00 20.38	A	C
ATOM	2213	0 7	VAL	303	42.687	69. 306	19.744	1.00 19.45	A	0 N
ATOM	2214		THR	304	41.562	71.102	18. 982 18. 882	1.00 20.04 1.00 19.30	A A	N C
ATOM	2215		THR	304	40. 302 39. 494	70. 394 70. 546	20. 191	1.00 19.30	A	C
ATOM	2216		THR THR	304 304	39. 494 40. 256	70. 024	21. 287	1.00 20.19	A	ŏ
ATOM ATOM	$\begin{array}{c} 2217 \\ 2218 \end{array}$		THR	304	38. 168	69. 812	20.090	1.00 17.51	A	С
ATOM	2219		THR	304	39. 467	70. 930	17.733	1.00 18.56	A	C
ATOM	2220		THR	304	39. 185	72.127	17.674	1.00 19.32	A	0
ATOM	2221		TRP	305	39. 082	70.042	16.819	1.00 18.08	A	N
ATOM	2222		TRP	305	38. 243	70.422	15.681	1.00 16.88	A	C C
ATOM	2223		TRP	305	38. 332	69. 394 69. 464	14. 546 13. 745	1.00 13.92 1.00 13.82	A A	C
ATOM	2224		TRP TRP	305 305	39. 581 39. 815	70. 296	12. 606	1.00 13.04	A	č
ATOM ATOM	2225 2226		TRP	305	41. 143	70.068	12. 189	1.00 13.12	Ā	Č .
ATOM	2227	CE3		305	39. 031	71.216	11.899	1.00 13.55	A	C
ATOM	2228	CD1		305	40.745	68. 781	13.967	1.00 13.51	A	C
ATOM	2229	NE1		305	41.688	69. 138	13.036	1.00 11.41	A	N
ATOM	2230	CZ2		305	41.704	70. 729	11.094	1.00 12.03	A	C
ATOM	2231	CZ3		305	39. 591	71.873 71.625	10.809 10.419	1.00 14.16 1.00 13.92	A A	C C
ATOM	2232	CH2	TRP	305 305	40. 914 36. 803		16. 155	1.00 16.35	A	č
ATOM ATOM	$\begin{array}{c} 2233 \\ 2234 \end{array}$		TRP	305 305	36. 368		16. 917	1.00 16.55	A	Ö
ATOM	2235		ALA	306	36.064		15. 704	1.00 16.10	A	N
ATOM	2236		ALA	306	34.661	71.620	16.079	1.00 17.20	Α	C
ATOM	2237		ALA	306	34. 336		16.384	1.00 18.47	A	C
ATOM	2238		ALA ·	306	33.770		14. 956	1.00 16.79	A	C
ATOM	2239		ALA	306	32. 829		15. 191 13. 733	1.00 18.46 1.00 18.36	A A	O N
ATOM	2240	N CA	THR THR	307 307	34. 076 33. 314		12. 564	1.00 18.30	A	C
ATOM ATOM	2241 2242	CA CB	THR	307	32. 387		12.072	1.00 18.43	Ä	č
ATOM	2243		THR	307	33. 178		11.473	1.00 20.76	A	0
ATOM	2244		THR	307	31. 593		13. 225	1.00 16.72	Α	С
ATOM	2245	C	THR	307	34. 299	70.778	11.442	1.00 20.34	A	C
ATOM	2246	0	THR	307	35. 494		11.689	1.00 22.05	A	0
ATOM	2247	N	GLN	308	33. 798		10. 213	1.00 20.11	A	N
ATOM	2248		GLN	308	34.640		9. 066 7. 866	1.00 19.71 1.00 19.44	A A	C C
ATOM	2249		GLN	308 308	33. 799 32. 845		8. 118	1.00 19.44	A	Č
ATOM ATOM	2250 2251	CD	GLN GLN	308	32. 645 33. 524		8. 557	1.00 23.81	A	č
ATOM	2252		GLN	308	32. 854		9.003	1.00 25.80		0
ATOM	2253		GLN	308	34. 848		8. 430	1.00 21.04		N
1110111	0				+					

·												(Continued)
FIG. 4-47												Continueu
							. .1					
ATOM	2254		GLN	308		35.440	71.616	8.653	1.00 19.			C
ATOM	2255		GLN	308		36. 421	71.501	7. 922	1.00 21.		ł	0
ATOM	2256		GLU	309		35. 022	72. 789	9.114	1.00 19.		<u> </u>	N C
ATOM	2257		GLU	309		35. 710	74. 019	8. 751	1.00 20.		4	C
ATOM	2258		GLU	309		34. 920	74. 764	7.685	1.00 21. 1.00 26.		A N	C C
ATOM	2259		GLU	309		34. 709	73. 971	6.419 5.413	1.00 20.		4 4	C
ATOM	2260		GLU	309		33.890	74. 731 74. 192	4. 305	1.00 25.		4	Ö
ATOM	2261 2262	0E1 0E2		309 309		33. 665 33. 471	75. 869	5. 736	1.00 31.		À	Ŏ
ATOM ATOM	2263		GLU	309		35. 924	74. 939	9. 932	1.00 21.		À	Č
ATOM	2264		GLU	309		36. 075	76. 152	9. 764	1.00 21.		Ā	0
ATOM	2265		ARG	310		35. 941	74. 360	11.125	1.00 20.		Ą	N
ATOM	2266		ARG	310		36. 133	75. 131	12.340	1.00 20.		A	C
ATOM	2267	CB	ARG	310		34.779	75.445	12.986	1.00 19.	87 A	A	C
ATOM	2268	CG	ARG	310		34.888	76.186	14.305	1.00 22.		A	С
ATOM	2269	CD	ARG	310		33. 519	76.630	14.786	1.00 21.		A	C
ATOM	2270		ARG	310	٤.	32. 952	77.605	13.870	1.00 20.		A	N
ATOM	2271	CZ	ARG	310		31.660	77. 884	13. 785	1.00 19.		A	C
ATOM	2272	NH1		310		30. 794	77. 261	14. 569	1.00 21.		A	N
ATOM	2273	NH2		310		31. 235	78. 776	12.902	1.00 21.		A	N
ATOM	2274	C	ARG	310		37.009	74. 346	13.304	1.00 19.		A	C
ATOM	2275	0	ARG	310		36. 701	73. 214	13.671	1.00 20.		A A	0 N
ATOM	2276	N	ILE	311		38. 108	74. 959 74. 320	13.710 14.619	1.00 17. 1.00 17.		A A	N C
ATOM ATOM	$\begin{array}{c} 2277 \\ 2278 \end{array}$	CA CB	ILE ILE	311 311		39. 044 40. 371	73. 991	13.859	1.00 17.		n. A	C
ATOM	2279	CG2		311		40. 982	75. 252	13. 305	1.00 14.		A.	C
ATOM	2280	CG1		311		41.358	73. 254	14. 765	1.00 17.		A	č
ATOM	2281	CD1		311		42. 589	72. 763	14.011	1.00 15.		A	č
ATOM	2282	Č	ILE	311		39. 283	75. 258	15.802	1.00 17.		Ã	Č
ATOM	2283	Ŏ	ILE	311		39. 267	76.481	15.649	1.00 17.		A	0
ATOM	2284	N	SER	312		39.461	74.692	16.988	1.00 16.		A	N
ATOM	2285	CA	SER	312		39. 694	75.517	18. 163	1.00 18.		A	C
ATOM	2286	CB	SER	312		38. 631	75. 244	19. 235	1.00 19.		A	C
ATOM	2287	0G	SER	312		39.008	74. 173	20.074	1.00 18.		A	0
ATOM	2288	C	SER	312		41.084	75. 269	18. 736	1.00 18.		A	Č
ATOM	2289	0	SER	312		41.552		18. 795	1.00 17.		A	0
ATOM	2290		LEU	313		41. 738	76.349	19.148	1.00 19.		A	N
ATOM	2291		LEU	313		43.080	76. 271	19.708	1.00 20.		A	C
ATOM	2292		LEU	313		44. 093	76.931	18.768	1.00 19.		A	C
ATOM	2293		LEU	313		44. 239	76. 409	17. 341	1.00 20.		A	C
ATOM	2294 2295	CD1		313		45. 480	77. 038 74. 892	16. 712 17. 351	1.00 19. 1.00 20.		A A	C C
ATOM ATOM	2296	CD2 C	LEU	313 313		44. 361 43. 172	76. 957	21.062	1.00 20.		A A	C
ATOM	2297	0	LEU	313		42. 608	78. 030	21. 265	1.00 21.		A.	0
ATOM	2298	N	GLN	314		43. 898	76. 333	21. 981	1.00 21.		A	N N
ATOM	2299	CA	GLN	314		44. 096	76.884	23. 308	1.00 22.		A	Ĉ
ATOM	2300	CB	GLN	314		43. 545	75. 935	24. 365	1.00 24.		A	Č
ATOM	2301	CG	GLN	314		42.033	75.860	24. 406	1.00 27.	30	A	С
ATOM	2302	CD	GLN	314		41.536	74.832	25. 401	1.00 29.	52 <i>i</i>	A	C

										(Continued)
					FΙ	G. 4	- 48			(00110111111111111111111111111111111111
ATOM	2303	0E1		314	41.827	74. 911	26. 598 24. 911	1.00 29.38 1.00 30.52	A	0 N
ATOM ATOM	2304 2305	NE2 C	GLN	314 314	40. 786 45. 584	73. 854 77. 099	23. 532	1.00 30.32	A A	C
ATOM	2306	Õ	GLN	314	46. 382	76. 176	23. 419	1.00 22.34	Ä	Ö
ATOM	2307	Ň	TRP	315	45. 954	78. 333	23.833	1.00 21.50	Α	N
ATOM	2308	CA	TRP	315	47. 343	78.667	24. 070	1.00 20.70	A	C
ATOM	2309	CB	TRP	315	47. 748	79. 873	23. 226	1.00 18.74	A	C
ATOM	2310	CC	TRP	315	47. 480	79. 711 79. 368	21. 746 20. 733	1.00 17.87 1.00 14.81	A A	C C
ATOM ATOM	$\frac{2311}{2312}$	CD2 CE2		315 315	48. 435 47. 764	79. 419	19. 491	1.00 14.81	A	č
ATOM	2312	CE3		315	49. 793	79. 029	20. 753	1.00 13.32	A	č
ATOM	2314			315	46. 299	79. 936	21.095	1.00 15.84	Ä	Č
ATOM	2315	NE1		315	46.463	79. 769	19. 742	1.00 13.87	Α	Ň
ATOM	2316	CZ2		315	48. 407	79. 147	18. 278	1.00 12.51	A	C
ATOM	2317	CZ3		315	50. 433	78. 760	19. 545	1.00 13.87	Α	C
ATOM	2318	CH2		315	49. 736	78. 822	18. 325	1.00 12.57	A	C
ATOM	2319	C	TRP	315	47.530	78. 976 79. 463	25. 545 26. 205	1.00 21.60 1.00 22.41	A A	C 0
ATOM ATOM	2320 2321	O N	TRP LEU	315 316	46. 615 48. 721	78. 689	26. 056	1.00 22.41	A	N N
ATOM	2322	CA	LEU	316	49. 033	78. 915	27. 458	1.00 22.64	A	Č
ATOM	2323	CB	LEU	316	49.034	77. 573	28. 192	1.00 22.20	Ä	č
ATOM	2324	CG	LEU	316	49.655	77.484	29.584	1.00 23.04	Α	С
ATOM	2325	CD1		316	48.953	78. 438	30. 530	1.00 24.08	Α	C
ATOM	2326	CD2		316	49. 557	76.049	30.085	1.00 19.71	A	C
ATOM	2327	C	LEU	316	50. 383	79.617	27. 618	1.00 24.44	A	C
ATOM	2328	0	LEU	316	51.392	79. 192	27. 046 28. 383	1.00 26.77 1.00 23.92	A	0
ATOM	2329 2330	N CA	ARG ARG	317 317	50.388 51.603	80. 704 81. 475	28. 630	1.00 23.92	A A	N C
ATOM ATOM	2331	CB	ARG	317	51. 265	82. 787	29. 337	1.00 25.72	A	č
ATOM	2332	CG	ARG	317	50. 490	83. 785	28. 504	1.00 26.56	A	č
ATOM	2333	CD	ARG	317	50. 187	85.012	29. 327	1.00 26.99	Α	C
ATOM	2334	NE	ARG	317	49. 796	86.141	28. 494	1.00 30.37	Α	N
ATOM	2335	CZ	ARG	317	49. 278	87. 269	28. 966	1.00 30.55	A	C
ATOM	2336	NH1	ARG	317	49. 082	87.414	30. 273	1.00 29.99	A	N
ATOM	2337		ARG	317	48. 972	88. 256	28. 132 29. 500	1.00 28.53	A	N C
ATOM	2338 2339	C 0	ARG ARG	317 317	52. 580 52. 175	80. 705 79. 920	30. 359	1.00 21.07 1.00 19.79	A A	0
ATOM ATOM	2340	N	ARG	318	53. 871	80. 941	29. 290	1.00 19.43	A	N
ATOM	2341	CA	ARG	318	54. 876	80. 259	30. 084	1.00 17.08	Ä	Ĉ
ATOM	2342	CB	ARG	318	56. 263	80. 850	29.845	1.00 15.15	A	Ċ
ATOM	2343	CG	ARG	318	57. 345	80.075	30. 564	1.00 13.58	Α	С
ATOM	2344	CD	ARG	318	58. 671	80. 165	29. 853	1.00 13.59	Α	С
ATOM	2345	NE	ARG	318	59. 687	79. 341	30. 504	1.00 11.13	A	N
ATOM	2346	CZ	ARG	318	60. 895	79. 135	30.001	1.00 10.46	A	C
ATOM	2347		ARG	318	61.220	79.694	28. 850	1.00 11.29 1.00 10.86	A A	N N
ATOM ATOM	2348 2349	NHZ C	ARG ARG	318 318	61.773 54.500	78. 378 80. 354	30. 642 31. 555	1.00 10.80	A	C .
ATOM	2350	0	ARG	318	54. 794	79. 448	32. 318	1.00 20.33	A	Ŏ.
ATOM	2351	N	ILE	319	53. 869	81.455	31.954	1.00 16.59	Ä	Ň

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										(Continued)
					FΙ	G. 4	- 49			(COIIIII aca)
ATOM	aara	CA	11.17	210	E9 906	81.607	33. 330	1.00 17.40	٨	С
ATOM ATOM	2352 2353	CA CB	ILE ILE	319 319	53. 396 53. 389		33. 776	1.00 17.40	A A	Č
ATOM	2354	CG2		319	52. 720		35. 128	1.00 17.19	A	č
ATOM	2355	CG1		319	54. 828		33. 878	1.00 19.57	A	č
ATOM	2356		ILE	319	55. 712		34. 787	1.00 19.56	A	Č
ATOM	2357	Č	ILE	319	51.972		33. 251	1.00 17.56	Α	С
ATOM	2358	Ŏ	ILE	319	51.012		33.067	1.00 18.71	Α	0
ATOM	2359		GLN	320	51.870		33. 381	1.00 16.94	Α	N
ATOM	2360	CA	GLN	320	50.623		33. 246	1.00 16.12	A	C
ATOM	2361	CB	GLN	320	50. 939		33. 420	1.00 14.59	A	C
ATOM	2362	CG	GLN	320	52.000		32. 444	1.00 12.17	A	C
ATOM	2363	CD	GLN	320	52. 304		32. 570	1.00 10.79	A	C
ATOM	2364		GLN	320	51. 431	74. 734	32. 403	1.00 12.70	A	0
ATOM	2365		GLN	320	53. 554		32.860	1.00 13.71	A	N
ATOM	2366	C	GLN	320	49. 368		34. 038	1.00 16.32	A	C
ATOM ATOM	2367 2368	O N	GLN ASN	320 321	48. 645		34. 472 34. 207	1.00 14.51 1.00 18.37	A A	O N
ATOM	2369	CA	ASN	321	49. 079 47. 871	81.010	34. 201	1.00 10.37	A	C
ATOM	2370	CB	ASN	321	48. 226		36. 203	1.00 20.21	A	č
ATOM	2371	CG	ASN	321	48. 776		35. 925	1.00 23.59	Ä	č
ATOM	2372	0D1		321	49. 166		34. 804	1.00 22.35	Ä	Ö
ATOM	2373	ND2		321	48. 801	83. 975	36. 980	1.00 27.82	Ä	N
ATOM	2374	C	ASN	321	46.983		34.020	1.00 18.69	Α	С
ATOM	2375	0	ASN	321	46.095	82. 555	34.479	1.00 19.10	Α	0
ATOM	2376	N	TYR	322	47. 222		32.719	1.00 17.65	Α	N
ATOM	2377	CA	TYR	322	46. 482		31. 719	1.00 18.28	A	С
ATOM	2378	CB	TYR	322	47. 105		31. 599	1.00 18.09	A	C
ATOM	2379	CG	TYR	322	46.319		30. 792	1.00 20.14	A	C
ATOM	2380		TYR	322	46. 561	85. 037	29. 428	1.00 21.33	A	C
ATOM	2381	CE1		322	45. 843		28. 694	1.00 22.14	A	C
ATOM	2382 2383	CD2		322	45. 340		31.401	1.00 20.00	A	C
ATOM ATOM	2384	CE2 CZ	TYR	$\begin{array}{c} 322 \\ 322 \end{array}$	44. 624 44. 876		30. 681 29. 334	1.00 19.18 1.00 21.74	A A	C C
ATOM	2385	OH ·	TYR	322	44. 163		28. 638	1.00 21.14	A	0
ATOM	2386	C	TYR	322	46. 518		30. 363	1.00 18.70	A	Č
ATOM	2387	ŏ	TYR	322	47. 583		29. 764	1.00 18.36	A	Ŏ.
ATOM	2388	Ň	SER	323	45. 351	81. 318	29. 896	1.00 17.43	A	Ň
ATOM	2389	CA	SER	323	45. 237		28. 612	1.00 17.45	Ā	Ċ
ATOM	2390	CB	SER	323	44.871		28.806	1.00 16.45	A	Ċ
ATOM	2391	0G	SER	323	43.662		29. 535	1.00 17.51	Α	0
ATOM	2392	C	SER	323	44. 163	81.320	27.777	1.00 17.88	Α	С
ATOM	2393	0	SER	323	43. 250		28. 314	1.00 18.20	A	0
ATOM	2394	N	VAL	324	44. 277		26. 461	1.00 18.44	A	Ŋ
ATOM	2395		VAL	324	43. 309		25. 555	1.00 18.83	A	C
ATOM	2396		VAL	324	43. 925		24. 800	1.00 19.32	A	C
ATOM	2397	CG1		324	42.944		23. 760	1.00 18.46	A	C
ATOM	2398	CG2		324	44. 290		25. 785	1.00 18.78	A	C
ATOM ATOM	2399		VAL	324	42. 839 43. 631		24. 534	1.00 18.47 1.00 18.75	A A	C 0
ATOM	2400	0	VAL	324	40. 091	79. 985	24. 036	1.00 10.10	A	U

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										(Con	tinued)
					FI	G. 4	- 50				
ATOM	2401	N	MET	325	41.549	80.772	24. 231	1.00 17.		N	
ATOM	2402	CA	MET	325	41.046	79.832	23.245	1.00 17.0		Č	
ATOM	2403	CB	MET	325	39.832	79.062	23.769	1.00 19.		C	
ATOM	2404	CG	MET	325	39. 272	78.043	22.774	1.00 20.		C	
ATOM	2405	SD	MET	325	37. 681	77.304	23. 268	1.00 23.		S	
ATOM	2406		MET	325	38. 209	75. 734	23.896	1.00 24.		C	
ATOM	2407		MET	325	40.641	80.584	21.999	1.00 18.		C	
ATOM	2408		MET	325	39. 932	81.583	22.076	1.00 16.		0	
ATOM	2409		ASP	326	41.114	80.118	20.852	1.00 18.		Ņ	
ATOM	2410		ASP	326	40.749	80. 738	19.595	1.00 20.		C	
ATOM	2411		ASP	326		81.158	18. 797	1.00 22.4		C C	
ATOM	2412		ASP	326		82.638	18.970	1.00 26.0 1.00 26.0		0	
ATOM	2413	OD1		326	41.511	83. 384	19. 547 18. 518	1.00 28.		0	
ATOM	2414	OD2		326	43. 415 39. 924	83. 063 79. 739	18. 800	1.00 28.		Č	
ATOM	2415		ASP ASP	326 326	40. 254	78. 563	18. 729	1.00 21.		ŏ	
ATOM ATOM	2416 2417		ILE	327	38. 832	80. 208	18. 223	1.00 20.		Ň	
ATOM	2418		ILE	327	37. 980	79. 355	17. 419	1.00 22.		Ċ	
ATOM	2419	CB	ILE	327	36. 529	79. 393	17. 941	1.00 20.		č	
ATOM	2420	CG2		327	35.600	78.697	16.985	1.00 19.		C	
ATOM	2421	CG1		327	36. 483	78.691	19.305	1.00 21.		C	
ATOM	2422	CD1		327	35. 164	78.766	20.006	1.00 20.		· C	
ATOM	2423	C	ILE	327	38. 113	79.908	16.015	1.00 23.	66 A	C	
ATOM	2424	0	ILE	327	37.625	80.984	15.716	1.00 26.		0	
ATOM	2425	N	CYS	328	38. 804	79. 162	15. 161	1.00 26.		N	
ATOM	2426	CA	CYS	328	39.069	79.608	13.805	1.00 26.		C	
ATOM	2427	C	CYS	328	38. 274	78. 890	12. 721	1.00 27.		C	
MOTA	2428	0	CYS	328	38. 168	77. 663	12.705	1.00 27.		0	
ATOM	2429	CB	CYS	328	40. 564	79. 481	13.547	1.00 27.		C	
ATOM	2430	SG	CYS	328	41.567	79.984	14.986	1.00 28.		S	
ATOM	2431	N	ASP	329	37. 729	79.686	11.807	1.00 26. 1.00 26.		N C	
ATOM	2432		ASP	329	36. 913	79. 198 79. 969	10. 710 10. 690	1.00 26.		Č	
ATOM	2433 2434	CB CG	ASP ASP	329 · 329	35. 595 34. 684		11.842	1.00 24.		Č	
ATOM ATOM	2435		ASP	329 329	35. 181	79. 407	12.969	1.00 20.		Õ	
ATOM	2436		ASP	329	33. 460	79. 493	11.625	1.00 28.		ő	•
ATOM		C			37.613		9. 367	1.00 28.			
ATOM	2438	ŏ	ASP	329	38. 314	80. 334	9. 120	1.00 29.		ŏ	
ATOM	2439	Ň	TYR	330	37. 416	78. 371	8. 492	1.00 29.		N	
ATOM	2440	CA	TYR	330	38.027	78.411	7.173	1.00 29.		С	
ATOM	2441	CB	TYR	330	38.011	77.019	6.542	1.00 30.		С	
ATOM	2442	CG	TYR	330	38. 597	76.980	5. 151	1.00 31.		С	
ATOM	2443	CD1	TYR	330	39.919	77. 367	4.919	1.00 32.		C	
ATOM	2444	CE1	TYR	330	40.460	77. 341	3.641	1.00 32.		C	
ATOM	2445		TYR	330	37. 832	76. 561	4.066	1.00 32.		C	
ATOM	2446		TYR	330	38. 364	76. 526	2. 779	1.00 32.		C	
ATOM	2447	CZ	TYR	330	39.676	76. 920	2.574	1.00 33.		C	
ATOM	2448	OH	TYR	330	40. 193	76.914	1. 299	1.00 34.		0	
ATOM	2449	C	TYR	330	37. 314	79. 387	6.243	1.00 30.	14 A	C	

(Continued)

					FΙ	G. 4	- 51			
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2450 2451 2452 2453 2454 2455 2456 2457 2458 2461 2462 2463 2464 2465 2466 2467 2468 2471 2472 2473 2474 2475 2476 2477 2478	CD OE1 OE2 C O N CA CB OG C O N CA CB	ASP ASP GLU GLU GLU GLU GLU GLU GLU SER SER SER SER SER SER SER SER SER	330 331 331 331 331 331 331 332 332 332 332	F I 36. 098 38. 074 37. 511 38. 191 37. 573 37. 570 37. 084 37. 750 36. 690 36. 755 35. 388 35. 234 33. 869 33. 494 33. 175 37. 231 37. 846 36. 968 37. 388 36. 445 36. 669 38. 826 39. 324 39. 496 40. 883 40. 995 40. 954 41. 722	79. 313 80. 308 81. 262 82. 618 83. 661 83. 455 84. 684 80. 696 80. 730 80. 170 79. 562 78. 970 77. 771 77. 534 80. 465 79. 982 81. 764 82. 652 83. 858 84. 795 83. 135 83. 838 82. 761 83. 163 84. 180 83. 536 81. 947	- 5 1 6. 058 5. 666 4. 730 4. 862 3. 956 2. 724 4. 479 3. 336 2. 817 2. 743 1. 426 1. 080 -0. 354 -0. 620 -1. 807 0. 358 0. 293 -0. 655 0. 375 -0. 704 -0. 814 0. 223 -0. 577 -1. 448 0. 506 0. 708 1. 844 3. 108 1. 058	1. 00 28. 65 1. 00 31. 49 1. 00 36. 63 1. 00 39. 35 1. 00 40. 70 1. 00 42. 41 1. 00 35. 29 1. 00 36. 11 1. 00 37. 77 1. 00 43. 60 1. 00 47. 15 1. 00 48. 97 1. 00 48. 40 1. 00 38. 19 1. 00 39. 73 1. 00 38. 87 1. 00 38. 97 1. 00 38. 49 1. 00 37. 74 1. 00 38. 52 1. 00 38. 49 1. 00 38. 49 1. 00 38. 52 1. 00 38. 49 1. 00 38. 50 1. 00 38. 48 1. 00 38. 50 1. 00 38. 48 1. 00 38. 59 1. 00 38. 48 1. 00 38. 59	. AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2475 2476 2477 2478 2479 2480 2481 2482 2483 2484 2485 2486 2487 2488 2489	CA CB OG C O N CA C O N CA CB CC CD NE	SER SER SER SER GLY GLY GLY ARG ARG ARG ARG	334 334 334 335 335 335 335 336 336 336 336	40. 883 40. 995 40. 954 41. 722 42. 941 41. 064 41. 797 42. 579 43. 574 42. 128 42. 783 43. 066 43. 957 44. 807 44. 010	83. 163 84. 180 83. 536 81. 947 82. 029 80. 817 79. 620 79. 872 79. 201 80. 855 81. 197 82. 696 83. 232 84. 374 85. 359	0. 708 1. 844 3. 108 1. 058 1. 148 1. 263 1. 620 2. 894 3. 172 3. 666 4. 919 4. 991 3. 884 4. 416 5. 147	1. 00 37. 49 1. 00 38. 50 1. 00 38. 48 1. 00 35. 98 1. 00 35. 13 1. 00 35. 71 1. 00 35. 19 1. 00 35. 61 1. 00 33. 15 1. 00 36. 78 1. 00 42. 04 1. 00 48. 92	A A A A A A A A A A A A A A A A A A A	C C O C O N C C C C N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2490 2491 2492 2493 2494 2495 2496 2497 2498		ARG ARG ARG ARG TRP TRP TRP	336 336 336 336 337 337 337	44. 510 45. 805 43. 718 41. 935 40. 763 42. 544 41. 869 42. 616 42. 460	86. 192 86. 159 87. 057 80. 801 80. 449 80. 869 80. 531 79. 403 78. 074	6. 055 6. 348 6. 675 6. 118 5. 981 7. 294 8. 533 9. 248 8. <u>56</u> 1	1. 00 50. 76 1. 00 52. 08 1. 00 52. 33 1. 00 30. 26 1. 00 29. 07 1. 00 26. 94 1. 00 24. 29 1. 00 19. 88 1. 00 15. 10	A A A A A A	C N C O N C C

				FIC 4-59	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2499 2500 2501 2502 2503 2504 2505 2506 2507 2508 2511 2512 2513 2514 2515 2516 2517 2518	CD2 TRP CE2 TRP CE3 TRP CD1 TRP NE1 TRP CZ2 TRP CZ3 TRP CH2 TRP C TRP O TRP N ASN CA ASN CB ASN CG ASN OD1 ASN ND2 ASN C ASN O ASN N CYS CA CYS	337 337 337 337 337 337 337 338 338 338	FIG. 4 - 52 41. 481 77. 077 8. 861 1. 00 9. 80 A 41. 651 76. 026 7. 927 1. 00 9. 92 A 40. 475 76. 970 9. 825 1. 00 7. 74 A 43. 173 77. 601 7. 485 1. 00 12. 90 A 42. 688 76. 369 7. 099 1. 00 9. 82 A 40. 849 74. 885 7. 935 1. 00 9. 71 A 39. 675 75. 836 9. 832 1. 00 7. 79 A 39. 866 74. 808 8. 894 1. 00 10. 33 A 41. 783 81. 758 9. 425 1. 00 24. 55 A 42. 794 82. 360 9. 766 1. 00 26. 73 A 40. 570 82. 128 9. 806 1. 00 25. 00 A 40. 381 83. 296 10. 648 1. 00 26. 17 A 39. 464 84. 300 9. 949 1. 00 28. 44 A 40. 016 84. 761 8. 612 1. 00 30. 42 A 39. 320 84. 711 7. 596 1. 00 32. 04 A 41. 271 85. 217 8. 606 1. 00 28. 33 A 39. 810 82. 958 12. 012 1. 00 25. 29 A 40. 293 83. 668 13. 023 1. 00 25. 00 A 39. 833 83. 482 14. 389 1. 00 24. 73	(Continued) C C C C N C C C C C C C O N C C C C C
ATOM	2519	C CYS	339	39. 289 84. 829 14. 888 1. 00 22. 42 A	C
ATOM	2520	O CYS	339	40. 051 85. 717 15. 249 1. 00 21. 56 A	0
ATOM	2521	CB CYS	339	40. 992 83. 014 15. 285 1. 00 25. 93 A	C
ATOM	2522	SG CYS	339	42. 199 81. 865 14. 526 1. 00 29. 61 A	S
ATOM	2523	N LEU	340	37. 968 84. 978 14. 889 1. 00 22. 38 A 37. 333 86. 212 15. 347 1. 00 20. 83 A	N
ATOM	2524	CA LEU	340		C
ATOM	2525	CB LEU	340	35. 839 86. 185 15. 069 1. 00 19. 89 A	C
ATOM	2526		340	35. 364 86. 201 13. 626 1. 00 19. 14 A	C
ATOM	2527	CD1 LEU	340	33. 877 85. 883 13. 593 1. 00 19. 65 A	C
ATOM	2528	CD2 LEU	340	35. 647 87. 551 13. 012 1. 00 19. 21 A	C
ATOM	2529	C LEU	340	37. 521 86. 406 16. 835 1. 00 20. 16 A	C
ATOM	2530	O LEU	340	37. 337 85. 478 17. 615 1. 00 20. 80 A	0
ATOM	2531	N VAL	341	37. 866 87. 625 17. 225 1. 00 20. 46 A 38. 066 87. 949 18. 627 1. 00 20. 11 A	N
ATOM	2532	CA VAL	341		C
ATOM	2533	CB VAL	341	38. 536 89. 399 18. 786 1. 00 21. 45 A 38. 972 89. 647 20. 221 1. 00 22. 38 A	C
ATOM	2534	CG1 VAL	341		C
ATOM	2535	CG2 VAL	341	39. 688 89. 672 17. 819 1. 00 24. 28 A 36. 770 87. 749 19. 403 1. 00 18. 51 A	C
ATOM	2536	C VAL	341		C
ATOM	2537 2538	0 VAL	341 342	36. 785 87. 423 20. 585 1. 00 17. 77 A 35. 644 87. 941 18. 731 1. 00 19. 68 A	O N
ATOM ATOM	2539	CA ALA	342	34. 345 87. 756 19. 370 1. 00 19. 64 A	C C
ATOM	2540	CB ALA	342	33. 228 88. 125 18. 407 1. 00 18. 89 A	C
ATOM	2541	C ALA	342	34. 177 86. 302 19. 829 1. 00 19. 19 A	
ATOM	2542	O ALA	342	33. 245 85. 987 20. 580 1. 00 18. 12 A	O
ATOM	2543	N ARG	343	35. 078 85. 422 19. 384 1. 00 16. 06 A	N
ATOM	2544 2545	CA ARG CB ARG	343 343	35.008 84.017 19.766 1.00 16.37 A 34.962 83.138 18.521 1.00 18.14 A	C
ATOM ATOM ATOM	2546 2547	CG ARG CD ARG	343 343	33. 726 83. 390 17. 687 1. 00 20. 31 A 33. 803 82. 695 16. 357 1. 00 21. 82 A	C

(Continued)

					FI	G. 4	- 53			(C01
ATOM	0.540	NE	ARG	343	32. 615	82. 969	15. 561	1.00 23.94	A	N
ATOM	2548 2549	CZ	ARG	343	32. 373	82. 415	14. 383	1.00 26.14	A	Č
ATOM ATOM	2550		ARG	343	33. 242	81.559	13. 864	1.00 28.42	A	Ň
ATOM	2551		ARG	343	31. 256	82. 703	13. 734	1.00 30.23	A	N
ATOM	2552	C	ARG	343	36.164	83. 603	20.650	1.00 17.09	A	Ċ
ATOM	2553	Ö	ARG	343	36. 275	82. 452	21.057	1.00 16.76	Ä	Ŏ
ATOM	2554	Ň	GLN	344	37. 030	84. 553	20. 955	1.00 18.05	Ā	Ň
ATOM	2555	CA	GLN	344	38. 175	84. 267	21.791	1.00 18.90	Α	C
ATOM	2556	CB	GLN	344	39. 191	85. 385	21.645	1.00 18.03	Α	С
ATOM	2557	CG	GLN	344	40. 585	85.012	22.038	1.00 17.99	Α	C C
ATOM	2558	CD	GLN	344	41.571	86.088	21.657	1.00 18.02	Α	
ATOM	2559	0E1	GLN	344	41.711	87.089	22. 353	1.00 17.71	Α	0
ATOM	2560	NE2	GLN	344	42. 246	85.897	20. 527	1.00 17.42	Α	N
ATOM	2561	С	GLN	344	37. 708	84.170	23. 234	1.00 19.61	Α	C
ATOM	2562	0	GLN	344	37.069	85.087	23. 730	1.00 21.89	A	0
ATOM	2563	N	HIS	345	38.013	83.057	23. 897	1.00 18.47	A	N
ATOM	2564	CA	HIS	345	37.624	82.868	25. 287	1.00 17.92	A	C
ATOM	2565	CB	HIS	345	36. 786	81.600	25. 453	1.00 16.07	A	C C
ATOM	2566	CG	HIS	345	35. 478	81.641	24. 726	1.00 15.01	A	C
ATOM	2567		HIS	345	34. 223	81.895	25. 164	1.00 14.43	A	C
ATOM	2568		HIS	345	35. 371	81.420	23. 369	1.00 15.56 1.00 12.57	A	N C
ATOM	2569		HIS HIS	$\begin{array}{c} 345 \\ 345 \end{array}$	34. 108 33. 390	81.535 81.823	23. 002 24. 073	1.00 12.57	A A	N
ATOM ATOM	2570 2571	C.	HIS	345	38. 854	82. 789	26. 172	1.00 14.20	A	C
ATOM	2572	0	HIS	345 345	39. 839	82. 129	25. 825	1.00 13.04	A	Õ
ATOM	2573	N	ILE	346	38. 790	83. 460	27. 319	1.00 20.11	A	N
ATOM	2574	CA	ILE	346	39. 899	83. 501	28. 264	1.00 21.08	Ä	Č
ATOM	2575	CB	ILE	346	40. 135	84. 928	28. 760	1. 00 20. 44	Ä	č
ATOM	2576		ILE	346	41. 357	84. 972	29.667	1.00 20.95	Ä	Č
ATOM	2577		ILE	346	40. 338	85.860	27.572	1.00 19.87	Ā	Č
ATOM	2578		ILE	346	40.466	87. 298	27.978	1.00 22.20	Α	C
ATOM	2579	С	ILE	346	39.657	82.624	29.482	1.00 23.76	Α	С
ATOM	2580	0	ILE	346	38. 535	82.537	29.975	1.00 24.67	Α	0
ATOM	2581	N	GLU	347	40. 714	81.976	29.967	1.00 25.01	Α	N
ATOM	2582	CA	GLU	347	40. 601	81.123	31.141	1.00 28.30	Α	C
ATOM	2583	CB	GLU	347	40. 459	79.656	30. 733	1.00 26.51	A	C
ATOM	2584	CG	GLU	347	40.089	78. 740	31.891	1.00 27.38	A	C
ATOM	2585	CD	GLU	347	40. 169	77. 268	31.527	1.00 29.51	A	C
ATOM	2586		GLU	347	39. 877	76. 936	30. 359	1.00 29.48	A	0
ATOM	2587		GLU	347	40.511	76. 439	32. 405	1.00 29.57	A	0
ATOM	2588	C	GLU	347	41.836	81. 288	32. 021	1.00 30.87	A	C
ATOM	2589 2590	O N	GLU MET	347 348	42.865	80.661	31.777 33.044	1.00 33.35 1.00 32.50	A ^	0
ATOM ATOM	2591	CA	MET	348	41. 741 42. 877	82. 131 82. 347	33. 926	1.00 32.30	A A	N C
ATOM	2592	CB	MET	348	43. 215	83. 843	34. 002	1.00 34.40	A	C
ATOM	2593	CG	MET	348	42. 168	84. 723	34.661	1.00 41.62	Ä	
ATOM	2594	SD	MET	348	42. 100	86. 340	33. 825	1.00 48.03	A	C S
ATOM	2595	CE	MET	348	43. 541	87. 158	34. 341	1.00 46.60	A	č
ATOM	2596	C	MET	348	42.628	81.784	35. 315	1.00 33.55	Ä	Č
112 01-2		-				101				-

					(Continued)
				FIG. 4-54	
ATOM	2597	0 MET	348	41.656 81.070 35.541 1.00 34.35 A	0 N
ATOM	2598	N SER	349	43. 534 82. 085 36. 235 1. 00 32. 30 A	N C
ATOM	2599	CA SER	349	43. 428 81. 623 37. 612 1. 00 31. 26 A 43. 961 80. 197 37. 744 1. 00 31. 22 A	Ċ
ATOM	2600	CB SER	349	10.001	0
ATOM	2601	OG SER	349		Č
ATOM	2602	C SER	349		ŏ
ATOM	2603	O SER	349	45. 355 82. 950 38. 113 1. 00 31. 25 A 43. 682 82. 962 39. 611 1. 00 30. 83 A	N
MOTA	2604	N THR CA THR	350 350	44. 340 83. 896 40. 516 1. 00 28. 43 A	Ċ
ATOM ATOM	2605 2606	CB THR	350	43. 325 84. 938 41. 027 1. 00 28. 93 A	Č
ATOM	2607	OG1 THR	350	42.251 84.268 41.703 1.00 27.68 A	0
ATOM	2608	CG2 THR	350	42. 751 85. 733 39. 864 1. 00 27. 87 A	С
ATOM	2609	C THR	350	44.971 83.198 41.714 1.00 27.14 A	C
ATOM	2610	0 THR	350	45. 781 83. 786 42. 431 1. 00 27. 62 A	0
ATOM	2611	N THR	351	44.610 81.936 41.913 1.00 25.72 A	Ŋ
ATOM	2612	CA THR	351	45. 109 81. 161 43. 035 1. 00 24. 77 A	C
ATOM	2613	CB THR	351	43. 945 80. 536 43. 786 1. 00 25. 52 A	C
ATOM	2614	OG1 THR	351	43. 166 79. 746 42. 877 1. 00 24. 95 A	0
ATOM	2615	CG2 THR	351	43. 069 81. 617 44. 385 1. 00 24. 61 A	C
ATOM	2616	C THR	351	46. 081 80. 047 42. 659 1. 00 25. 48 A	C 0
ATOM	2617	0 THR	351	46.648 79.392 43.535 1.00 25.57 A 46.261 79.825 41.361 1.00 25.19 A	N N
ATOM	2618	N GLY	352		Č
ATOM	2619	CA GLY	352	47. 170 78. 786 40. 909 1. 00 24. 62 A 47. 371 78. 797 39. 403 1. 00 24. 61 A	Č
ATOM	2620	C GLY O GLY	$\begin{array}{c} 352 \\ 352 \end{array}$	47. 417 79. 853 38. 774 1. 00 25. 15 A	ŏ
ATOM	2621 2622	N TRP	353	47. 499 77. 612 38. 825 1. 00 23. 36 A	Ň
ATOM ATOM	2623	CA TRP	353	47. 684 77. 470 37. 390 1. 00 21. 38 A	Ĉ
ATOM	2624	CB TRP	353	48. 631 76. 291 37. 116 1. 00 17. 49 A	C
ATOM	2625	CG TRP		48. 272 75. 023 37. 849 1. 00 16. 34 A	C
ATOM	2626	CD2 TRP		48. 587 74. 693 39. 209 1. 00 14. 04 A	C
ATOM	2627	CE2 TRP		48. 053 73. 409 39. 462 1. 00 14. 33 A	С
ATOM	2628	CE3 TRP		49. 270 75. 356 40. 238 1. 00 14. 55 A	Ċ
ATOM	2629	CD1 TRP		47.578 73.957 37.351 1.00 14.89 A	C
ATOM	2630	NE1 TRP		47. 445 72. 985 38. 311 1. 00 12. 84 A	N
ATOM	2631	CZ2 TRP		48. 180 72. 768 40. 709 .1. 00 14. 93 A	C
ATOM	2632	CZ3 TRP		49. 398 74. 719 41. 480 1. 00 15. 27 A	
ATOM	2633			48. 853 73. 436 41. 700 1. 00 15. 07 A	
ATOM	2634			46. 303 77. 236 36. 782 1. 00 22. 43 A 45. 307 77. 292 37. 495 1. 00 22. 69 A	
ATOM	2635				
ATOM	2636			46. 231 76. 990 35. 479 1. 00 22. 83 A 44. 944 76. 749 34. 836 1. 00 24. 15 A	
MOTA	2637			44. 818 77. 513 33. 498 1. 00 25. 09 A	
ATOM ATOM	2638 2639			43.610 77.006 32.718 1.00 24.29 A	
ATOM	2640			44. 673 79. 007 33. 762 1. 00 24. 71 A	_
ATOM	2641	C VAI		44. 799 75. 264 34. 569 1. 00 24. 96 A	_
ATOM	2642			45. 751 74. 628 34. 127 1. 00 26. 10 A	
ATOM	2643			43. 609 74. 722 34. 841 1. 00 24. 28 A	
ATOM	2644		355	43. 354 73. 303 34. 640 1. 00 22. 67 A	
ATOM	2645		355	44.040 72.457 35.696 1.00 22.77 A	C

				EIC 4-55	((Continued)
ATON	. 0040	O CIV	355	FIG. 4 - 55 44.743 72.989 36.548 1.00 22.56	A	0
ATOM	2646 2647	O GLY N ARG	356		A	N
ATOM ATOM	2648	CA ARG	356		A	C
ATOM ATOM	2649	CB ARG	356		Α	C
ATOM	2650	CG ARG	356	42, 495 68, 808 37, 122 1, 00 27, 84	Α	С
ATOM	2651	CD ARG	356	41.973 67.391 37.036 1.00 31.58	Α	С
ATOM	2652	NE ARG	356		Α	N
ATOM	2653	CZ ARG	356	39. 849 67. 607 38. 261 1. 00 37. 59	A	C
ATOM	2654	NH1 ARG	356	10.010 01.000 00.00=	A	N
ATOM	2655	NH2 ARG	356	00.000 0	A	N
ATOM	2656	C ARG	356	20.000 10.000	Ą	Ç
ATOM	2657	O ARG	356	46. 844 70. 508 37. 163 1. 00 28. 06	A	0
ATOM	2658	N PHE	357	46. 285 69. 940 35. 060 1. 00 23. 61	A	N
ATOM	2659	CA PHE	357	47.659 69.876 34.587 1.00 21.95	A	C
ATOM	2660	CB PHE	357	48. 029 68. 442 34. 205 1. 00 15. 99	A	C
ATOM	2661	CG PHE	357	48. 173 67. 524 35. 380 1. 00 12. 89	A	C C C
ATOM	2662	CD1 PHE	357	49. 361 67. 491 36. 115 1. 00 11. 73	A	C
ATOM	2663	CD2 PHE	357	47. 126 66. 693 35. 763 1. 00 10. 46	A	C
ATOM	2664	CE1 PHE	357	49. 507 66. 638 37. 216 1. 00 7. 55	A	C
ATOM	2665	CE2 PHE	357	47. 263 65. 838 36. 863 1. 00 11. 70	A	C
ATOM	2666	CZ PHE	357	48. 459 65. 811 37. 591 1. 00 6. 24 47. 775 70. 786 33. 377 1. 00 23. 17	A A	C
ATOM	2667	C PHE	357	= 1 · · · · = · · · · · · · · · · · · ·	A A	0
ATOM	2668	0 PHE	357		A	N N
ATOM	2669	N ARG	358		A	Č
ATOM	2670	CA ARG	358		A	č
ATOM	2671	CB ARG	358	47.156 71.297 30.396 1.00 19.30 46.496 69.991 30.011 1.00 21.15	A	č
ATOM	2672	CG ARG	358	46. 866 69. 613 28. 598 1. 00 24. 58	A	č
ATOM	2673	CD ARG	358	46. 293 68. 333 28. 205 1. 00 31. 68	Ä	Ň
ATOM	2674	NE ARG CZ ARG	358 358	46. 163 67. 924 26. 943 1. 00 34. 22	Ä	Ċ
ATOM	2675 2676	NH1 ARG	358	46.564 68.701 25.939 1.00 31.56	Ä	Ň
ATOM ATOM	2677	NH2 ARG	358	45. 640 66. 727 26. 687 1. 00 33. 62	A	N
ATOM	2678	C ARG	358	45. 081 72. 315 31. 313 1. 00 20. 40	A	C
ATOM	2679	O ARG	358	44. 168 71. 608 31. 734 1. 00 20. 47	A	0
ATOM	2680	N PRO	359	44. 840 73. 404 30. 570 1. 00 21. 33	Α	N
ATOM	2681	CD PRO	359	45. 785 74. 338 29. 940 1. 00 20. 09	Α	С
ATOM	2682	CA PRO	359	43. 455 73. 772 30. 254 1. 00 21. 44	Α	С
ATOM	2683	CB PRO	359	43. 624 74. 911 29. 264 1. 00 20. 76	Α	С
ATOM	2684	CG PRO	359	44. 907 75. 539 29. 713 1. 00 21. 86	A	C
ATOM	2685	C PRO	359	42.741 72.574 29.652 1.00 21.94	A	C
ATOM	2686	0 PRO	359	43. 314 71. 866 28. 827 1. 00 21. 94	A	0
ATOM	2687	N SER	360	41. 499 72. 350 30. 070 1. 00 22. 48	A	N
ATOM	2688	CA SER	360	40.723 71.208 29.596 1.00 24.26	A	C
ATOM	2689	CB SER	360	39. 501 70. 986 30. 497 1. 00 25. 29	A	C
ATOM	2690	OG SER	360	38. 505 71. 976 30. 283 1. 00 27. 66	A	0 .
ATOM	2691	C SER	360	40. 262 71. 280 28. 140 1. 00 25. 67	A	C
MOTA	2692	0 SER	360	40. 117 72. 359 27. 555 1. 00 25. 66	A	0 N
ATOM	2693		361	40.024 70.104 27.573 1.00 25.65 39.581 69.972 26.199 1.00 27.20	A	N C
ATOM	2694	CA GLU	361	39. 581 69. 972 26. 199 1. 00 27. 20	A	U

									(Continued)
				FIG	. 4 -	- 5 6			(Continued)
							1 00 00 05		0
ATOM	2695	CB GL			8. 540	25. 713	1.00 30.37	A	C
ATOM	2696	CG GI			57. 444	26. 683	1.00 36.42	A	C
ATOM	2697	CD GL			37. 226	27. 839	1.00 42.80 1.00 43.77	A A	C 0
ATOM	2698	OE1 GI			8. 002	28. 822	1.00 45.77	A	0
ATOM	2699	OE2 GI			66. 274 70. 324	27. 757 26. 052	1.00 40.00	A	C
ATOM	2700	C GI O GI			39. 955	26. 888	1.00 27.12		Õ
ATOM	2701 2702	N PF			71.061	24. 989	1.00 21.12	A	Ň
ATOM ATOM	2702	CD PF			71.837	24. 106	1.00 23.33	A	Ċ
ATOM	2704	CA PF			71.436	24. 767	1.00 22.45	A	č
ATOM	2705	CB PF			72. 714	23. 945	1.00 23.21	A	Č
ATOM	2706	CG PF			72. 437	23. 100	1.00 21.08	A	Ċ
ATOM	2707	C PF			70. 338	24.013	1.00 21.91	A	Ċ
ATOM	2708	0 PF			39. 582	23. 249	1.00 22.96	Α	0
ATOM	2709	N H			70. 259	24.245	1.00 21.59	Α	N
ATOM	2710	CA H			59. 280	23.596	1.00 19.88	Α	C
ATOM	2711	CB H	IS 363	32.868	38. 353	24.649	1.00 18.03	Α	C
ATOM	2712	CG H			57. 568	25.398	1.00 16.56	Α	C
ATOM	2713	CD2 H			57.880	26.489	1.00 16.19	A	C
ATOM	2714	ND1 H			36. 303	25.019	1.00 14.56	A	N
ATOM	2715	CE1 H			55.869	25. 843	1.00 14.60	A	<u>c</u>
ATOM	2716	NE2 H			66. 808	26. 744	1.00 16.65	A	N
ATOM	2717	C H			70. 081	22.903	1.00 20.84	A	C
ATOM	2718	0 H			70. 709	23. 564	1.00 20.84	A	0
ATOM	2719	N PI		•	70.075	21.573	1.00 19.87	A	N C
ATOM	2720	CA PI			70.832	20. 786 19. 470	1.00 18.84 1.00 18.67	A A	C C
ATOM	2721	CB PI			71. 310 72. 390	19. 629	1.00 18.07	A	Č
ATOM	2722 2723	CD1 PI			72. 096	20.117	1.00 17.51	A	Č
ATOM ATOM	2724	CD2 PI		32. 776	73. 708	19. 274	1.00 16.76	A	č
ATOM	2725	CE1 PI			73. 095	20. 246	1.00 16.92	Ä	č
ATOM	2726	CE2 PI			74. 711	19.401	1.00 16.24	A	č
ATOM	2727		HE 364		74. 404	19.886	1.00 16.59	A	Č
ATOM	2728		HE 364		70.046	20. 432	1.00 19.35	· A	Č
ATOM	2729		HE 364		68. 831	20.262	1.00 20.71	Α	0
ATOM	2730		HR 365		70.750	20.313	1.00 18.81	Α	N
ATOM	2731		HR 365	27. 805	70. 113	19.912	1.00 18.11	Α	С
ATOM	2732		HR 365		71.017	20.161	1.00 17.38	Α	С
ATOM	2733	OG1 T			71.991	19.119	1.00 22.40	Α	0
ATOM	2734	CG2 T			71.734	21.487	1.00 13.72	A	C
ATOM	2735		HR 365		69.954	18. 409	1.00 17.58	A	C
ATOM	2736		HR 365		70.650	17.824	1.00 16.70	A	0
ATOM	2737		EU 366		69.058	17. 784	1.00 19.74	A	N
ATOM	2738		EU 366		68. 799	16.350	1.00 19.89	A	C
ATOM	2739		EU 366		67. 923	15.860	1.00 19.49	A	C
ATOM	2740		EU 366		67.381	14. 431	1.00 19.63	A	C
ATOM	2741	CD1 L			66. 542	14. 282 14. 128	1.00 20.45 1.00 17.80	A	C .
MOTA	2742	CD2 L			66. 539 70. 017	14. 128	1.00 17.80	A A	Č
ATOM	2743	C L	EU 366	27. 503	10.011	10.400	1.00 21.11	n	V

				FIG. 4-57	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2744 2745 2746 2747 2748 2749 2750 2751 2752 2753 2754 2755 2756	0 LEU N ASP CA ASP CB ASP CG ASP 0D1 ASP 0D2 ASP C ASP 0 ASP N GLY CA GLY C GLY 0 GLY	366 367 367 367 367 367 367 367 368 368 368	28. 269 69. 989 14. 476 1. 00 24. 2 26. 764 71. 084 15. 722 1. 00 21. 2 26. 830 72. 261 14. 867 1. 00 22. 9 25. 567 73. 114 15. 005 1. 00 26. 0 25. 458 73. 796 16. 355 1. 00 29. 8 26. 469 73. 849 17. 094 1. 00 28. 7 24. 352 74. 296 16. 669 1. 00 31. 8 28. 047 73. 130 15. 139 1. 00 22. 7 28. 274 74. 122 14. 448 1. 00 25. 4 28. 818 72. 772 16. 155 1. 00 21. 0 30. 001 73. 541 16. 480 1. 00 18. 5 29. 740 74. 946 16. 987 1. 00 17. 4 30. 678 75. 690 17. 237 1. 00 17. 8	6 A N 5 A C 9 A C 2 A C 6 A O 8 A C 6 A O 6 A C 6 A O 2 A N 4 A C 2 A C 2 A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2757 2758 2759 2760 2761 2762 2763 2764 2765 2766	N ASN CA ASN CB ASN CG ASN OD1 ASN ND2 ASN C ASN O ASN N SER CA SER	369 369 369 369 369 369 369 370 370	28. 482 75. 324 17. 164 1. 00 17. 5 28. 196 76. 669 17. 647 1. 00 17. 8 26. 838 77. 129 17. 144 1. 00 18. 9 26. 797 77. 234 15. 649 1. 00 22. 4 27. 657 77. 871 15. 038 1. 00 23. 5 25. 798 76. 606 15. 038 1. 00 26. 5 28. 270 76. 838 19. 158 1. 00 16. 2 28. 185 77. 949 19. 665 1. 00 16. 4 28. 432 75. 742 19. 882 1. 00 15. 6 28. 533 75. 824 21. 330 1. 00 16. 3	2 A C 2 A C 1 A C 6 A O 2 A N 7 A C 4 A O 7 A N 4 A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2767 2768 2769 2770 2771 2772 2773 2774 2775	CB SER OG SER C SER O SER N PHE CA PHE CB PHE CG PHE CD1 PHE CD2 PHE	370 370 370 370 371 371 371 371 371	27. 145 75. 766 21. 971 1. 00 14. 44 26. 523 74. 518 21. 739 1. 00 14. 3 29. 381 74. 660 21. 797 1. 00 16. 66 29. 565 73. 701 21. 058 1. 00 18. 14 29. 910 74. 742 23. 014 1. 00 17. 09 30. 735 73. 660 23. 532 1. 00 16. 26 32. 194 73. 808 23. 062 1. 00 14. 83 32. 881 75. 062 23. 546 1. 00 11. 3 32. 799 76. 243 22. 818 1. 00 11. 03 33. 635 75. 050 24. 726 1. 00 11. 83	7 A O 6 A C 6 A O 8 A N 8 A C 8 A C 1 A C 7 A C 9 A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2781 2782 2783 2784 2785 2786 2787	CE1 PHE CE2 PHE CZ PHE C PHE O PHE N TYR CA TYR CB TYR CG TYR CD1 TYR CE1 TYR	371 371 371 371 372 372 372 372 372 372 372	33. 465 77. 409 23. 256 1. 00 12. 04 34. 302 76. 205 25. 178 1. 00 9. 92 34. 219 77. 383 24. 444 1. 00 9. 76 30. 703 73. 545 25. 048 1. 00 16. 26 30. 362 74. 495 25. 752 1. 00 16. 67 31. 053 72. 360 25. 536 1. 00 16. 67 31. 091 72. 089 26. 962 1. 00 16. 79 28. 892 70. 879 26. 914 1. 00 18. 47 28. 470 70. 744 25. 589 1. 00 16. 97 27. 129 70. 850 25. 255 1. 00 19. 91	A C A C B A C B A C B A C B A C B A C B A C C A N C A C C A C C A C C A C
ATOM ATOM ATOM ATOM ATOM	2789 2790 2791	CD2 TYR CE2 TYR CZ TYR OH TYR C TYR	372 372 372 372 372	27. 931 71. 124 27. 901 1. 00 18. 26 26. 592 71. 235 27. 581 1. 00 19. 23 26. 193 71. 097 26. 258 1. 00 21. 51 24. 860 71. 210 25. 944 1. 00 23. 32 32. 547 71. 977 27. 367 1. 00 18. 35	A C A C A C A O

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												(Con:	tinued)
					F	ΙG.	4	- 58				(001	umaca
A TO L	9709	۸	TVD	979	22 20	0 71	E E 77	96 571	1 00	20. 30	٨	0	
ATOM	2793	0 N	TYR	372	33. 38 32. 84		. 557 . 325	26. 571 28. 611		18. 89	A A	O N	
ATOM	2794	N CA	LYS LYS	373 373	34. 22		. 318	29. 071		19.69	· A	C	
ATOM ATOM	2795 2796		LYS	373	34. 22		. 541	28. 459		19.69	A	Č	
ATOM	2797	CG	LYS	373	36. 30		. 863	28. 889		20. 48	A	Č	
ATOM ATOM	2798	CD	LYS	373	36.65		. 193	28. 240		23. 59	A	č	
ATOM	2799	CE	LYS	373	38.04		. 703	28. 601		25. 15	A	č	
ATOM	2800	NZ	LYS	373	38. 10		. 196	28. 404		24. 26	Ä	N	
ATOM	2801	C	LYS	373	34. 27		. 369	30. 593		20. 26	A	Ċ	
ATOM	2802	ŏ	LYS	373	33. 47		. 050	31. 231		21.08	Ä	Ŏ.	
ATOM	2803	Ň	ILE	374	35. 21		. 634	31. 176		20. 43	A	Ň	
ATOM	2804	ĊA	ILE	374	35. 35		. 624	32.621		19.63	A	C	
ATOM	2805	CB	ILE	374	35.96		. 309	33. 123		19.72	Α	C	
ATOM	2806		ILE	374	36.10		. 361	34.650		19.46	Α	C	
ATOM	2807		ILE	374	35.09		. 128	32.667		19.17	Α	C	
ATOM	2808	CD1		374	35.65		. 753	33.079	1.00	15.57	Α	C	
ATOM	2809	C	ILE	374	36. 29	0 72	. 745	33.046	1.00	19.75	A .	C	
ATOM	2810	0	ILE	374	37.40		. 846	32.551		21.23	Α	0	
ATOM	2811	N	ILE	375	35.82		. 595	33. 951		20.12	Α	N	
ATOM	2812	CA	ILE	375	36.64		. 684	34. 456		20. 15	A	C	
ATOM	2813	CB	ILE	375	36.39		. 014	33. 700		20.38	A	C	
ATOM	2814		ILE	375	36.68		. 837	32. 215		20. 24	A	C	
ATOM	2815		ILE	375	34.96		. 488	33. 919		20. 36	A	C	
ATOM	2816		ILE	375	34.64		. 772	33. 186		21.00	A	C	
ATOM	2817	C	ILE	375	36.34		. 893	35. 929		21.63	A	C	
ATOM	2818	0	ILE	375	35. 28		. 512	36. 426		21.72	A	0	
ATOM	2819	N CA	SER	376	37. 30	1 /0	. 481	36.634		22. 04	A	N	
ATOM	2820	CA	SER	376	37.13		. 740	38. 051		23. 67 21. 76	A	C	
ATOM	2821 2822	CB OG	SER SER	376 376	38. 44 38. 33		. 228 . 411	38. 632 40. 022		26.97	A	C 0	
ATOM ATOM	2823	C	SER	376	36. 06		. 809	38. 210		24.46	A A	C	
ATOM	2824	0	SER	376	36.04		. 768	37. 445		27. 59	A	0	
ATOM	2825	N	ASN	377	35.16		. 659	39. 177		25.41	A	N	
ATOM	2826	ČA	ASN	377	34. 12		. 673	39. 356		26. 19	A	Č	
ATOM	2827	CB	ASN	377	32. 75		. 023	39. 602		25.06	A	č	
ATOM	2828	CG	ASN	377	32. 68		. 222	40. 894		22. 15	A	Č	
ATOM	2829		ASN	377	33. 56		. 294	41.750		23. 03	A	ŏ	
ATOM	2830		ASN	377	31.60		. 457	41.039		20.01	A	Ň	
ATOM	2831	C	ASN	377	34.44		. 685	40.456		28.48	Ā	Ċ	
ATOM	2832	0	ASN	377	35.57		. 733	40.960		29.51	A	Ō	
ATOM	2833	N	GLU	378	33.46		. 498	40.822		30.42	Ā	Ň	
ATOM	2834	CA	GLU	378	33.65		. 518	41.845	1.00	33. 25	Α	С	
ATOM	2835	CB	GLU	378	32.40	1 81	. 390	41.988		36.97	Α	С	
ATOM	2836	CG	GLU	378	32.30	0 82	. 505	40. 939		44. 33	Α	С	
ATOM	2837	CD	GLU	378	31.09		. 430	41.148		49. 20	Α	C	
ATOM	2838		GLU	378	29.94	6 82	. 970	40.972		51.65	Α	0	
ATOM	2839		GLU	378	31.31		. 619	41.489		50.97	A	0	
ATOM	2840	C	GLU	378	34.06		. 975	43. 208		32. 75	A	Ç	
ATOM	2841	0	GLU	378	34. 58	2 80	. 718	44. 040	1.00	33.80	Α	0	

				FIG. 4-59	(0	,011011111011,			
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2842 2843 2844 2845 2846 2847 2850 2851 2852 2853 2854 2855 2856 2857 2860 2861 2862 2863 2864 2865 2866 2867 2868 2869 2871	N GLU CA GLU CB GLU CG GLU OE1 GLU OE2 GLU OE2 GLU O GLY N GLY CA GLY O GLY N TYR CA TYR CB TYR CB TYR CCD1 TYR CCD2 TYR CCD2 TYR CCD2 TYR CCD2 TYR CCD3 TYR CCD4 TYR CCD6 TYR CCD7 TYR CCCC TYR CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	379 379 379 379 379 379 379 380 380 381 381 381 381 381 381 381 381 381 381	33. 842 78. 687 43. 436 1. 00 31. 75 34. 192 78. 070 44. 709 1. 00 31. 73 33. 083 77. 141 45. 182 1. 00 35. 37 31. 752 77. 788 45. 416 1. 00 40. 59 30. 678 76. 751 45. 677 1. 00 46. 30 30. 363 75. 976 44. 741 1. 00 48. 81 30. 159 76. 700 46. 815 1. 00 49. 11 35. 466 77. 252 44. 589 1. 00 30. 70 35. 952 76. 712 45. 578 1. 00 30. 56 35. 986 77. 136 43. 373 1. 00 29. 06 37. 203 76. 377 43. 171 1. 00 27. 19 36. 979 74. 931 42. 781 1. 00 27. 69 37. 935 74. 167 42. 662 1. 00 27. 62 35. 726 74. 540 42. 586 1. 00 26. 46 35. 434 73. 167 42. 191 1. 00 26. 78 34. 175 72. 671 42. 903 1. 00 26. 62 34. 394 72. 448 44. 379 1. 00 24. 99 34. 864 71. 225 44. 853 1. 00 24. 99 34. 864 71. 225 44. 853 1. 00 24. 93 35. 145 71. 035 46. 204 1. 00 26. 71 34. 202 73. 486 45. 296 1. 00 25. 27 34. 480 73. 312 46. 647 1. 00 26. 88 34. 955 72. 082 47. 097 1. 00 28. 08 35. 266 71. 909 48. 429 1. 00 28. 08 35. 266 71. 909 48. 429 1. 00 28. 94 35. 938 72. 147 40. 045 1. 00 28. 94 35. 938 72. 147 40. 045 1. 00 24. 97 35. 855 72. 003 38. 600 1. 00 22. 04 37. 057 71. 211 38. 081 1. 00 24. 10 38. 322 72. 045 38. 110 1. 00 24. 01	A A A A A A A A A A A A A A A A A A A	Continued) N C C C C C C C C C C C C C C C C C C			
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2871 2872 2873 2874 2875 2876 2877 2878 2889 2881 2882 2883 2884 2885 2886 2887 2888 2889 2890	N HIS CA HIS CB HIS CG HIS CD2 HIS ND1 HIS CE1 HIS NE2 HIS C HIS O HIS N ILE CA ILE	382 382 382 382 382 383 383 383 383 383	39. 606 71. 237 38. 141 1. 00 24. 10 40. 647 72. 083 38. 712 1. 00 23. 35 41. 178 73. 132 38. 096 1. 00 23. 31 40. 783 73. 449 36. 868 1. 00 21. 52 42. 052 73. 907 38. 738 1. 00 22. 46 34. 548 71. 359 38. 186 1. 00 20. 92 34. 189 70. 270 38. 645 1. 00 18. 12 33. 840 72. 068 37. 313 1. 00 20. 45 32. 545 71. 647 36. 813 1. 00 20. 33 31. 177 71. 797 38. 939 1. 00 20. 76 31. 177 71. 797 38. 939 1. 00 21. 75 30. 418 70. 661 39. 132 1. 00 21. 75 30. 374 70. 380 40. 422 1. 00 22. 91 31. 076 71. 291 41. 073 1. 00 22. 25 32. 404 71. 930 35. 330 1. 00 20. 36 33. 240 72. 608 34.	A A A A A A A A A A A A A A A A A A A	C N C N N C O N C C C C N C N C O N C C			

								(Continued)
				FIG. 4	- 60			
ATOM	2891	CG2 ILE	384	30.005 70.566	31.290	1.00 15.28	Α	С
ATOM	2892	CG1 ILE	384	30.928 69.097	33. 155	1.00 12.97	A	C
ATOM	2893	CD1 ILE	384	30. 093 67. 865	32.909	1.00 9.57	A	C ·
ATOM	2894	C ILE	384	30. 376 72. 898	33.028	1.00 19.30	A	C
ATOM	2895	0 ILE	384	29. 333 73. 198	33.605	1.00 18.50	A	0
ATOM	2896	N CYS	385	30. 950 73. 681	32.120	1.00 21.14	A	N
ATOM	2897	CA CYS	385	30. 349 74. 953	31.745	1.00 24.26	A	C
ATOM	2898	C CYS	385	29. 932 74. 887	30. 284	1.00 23.62	A	C
ATOM	2899	0 CYS	385	30. 654 74. 334	29. 464	1.00 23.61	A	0
ATOM	2900	CB CYS	385	31. 344 76. 106	31.958	1.00 27.85	A	C
ATOM	2901	SG CYS	385	30. 561 77. 640	32. 569	1.00 37.75	A	S
ATOM	2902	N TYR CA TYR	386	28. 760 75. 440 28. 237 75. 470	29. 973	1.00 23.26	A	N C
ATOM	2903 2904	CA TYR CB TYR	386 386	28. 237 75. 470 26. 726 75. 271	28. 609 28. 612	1.00 21.88 1.00 21.89	A	C
ATOM ATOM	2904	CG TYR	386	26. 120 75. 183	27. 228	1.00 21.69	A A	C
ATOM	2906	CD1 TYR	386	24. 912 75. 825	26. 930	1.00 23.46	A	C C
ATOM	2907	CE1 TYR	386	24. 323 75. 712	25.665	1.00 23.33	A	C
ATOM	2908	CD2 TYR	386	26. 728 74. 424	26. 223	1.00 22.70	A	Č
ATOM	2909	CE2 TYR	386	26. 144 74. 299	24. 956	1.00 23.04	A	č
ATOM	2910	CZ TYR	386	24. 943 74. 946	24. 686	1.00 24.39	Ä	č
ATOM	2911	OH TYR	386	24. 358 74. 823	23. 449	1.00 23.13	Ä	Ö
ATOM	2912	C TYR	386	28. 549 76. 816	27.962	1.00 22.02	Ā	Č
ATOM	2913	0 TYR	386	28. 187 77. 868	28.493	1.00 22.52	Α	0
ATOM	2914	N PHE	387	29. 201 76. 775	26.806	1.00 21.19	Α	N
ATOM	2915	CA PHE	387	29.582 77.988	26.080	1.00 19.95	Α	C
ATOM	2916	CB PHE	387	31.087 77.987	25.781	1.00 17.05	Α	C
ATOM	2917	CG PHE	387	31.970 78.222	26.973	1.00 14.01	Α	C
ATOM	2918	CD1 PHE	387	32. 547 79. 469	27. 185	1.00 9.81	A	С
ATOM	2919	CD2 PHE	387	32. 293 77. 178	27. 835	1.00 11.20	A	Č
ATOM	2920	CE1 PHE	387	33. 440 79. 672	28. 231	1.00 9.80	A	C
ATOM	2921	CE2 PHE	387	33. 185 77. 376	28. 885	1.00 10.91	Ą	C
ATOM	2922	CZ PHE	387	33. 762 78. 626	29.082	1.00 9.32	A	C
ATOM	2923	C PHE	387	28. 888 78. 153	24. 727	1.00 20.94	A	C
ATOM	2924 2925	0 PHE	387 388	28. 552 77. 180	24. 055	1.00 19.77	A	0
ATOM ATOM	2926	N GLN CA GLN	388	28. 706 79. 406 28. 151 79. 742	24. 332	1.00 21.79	A	N C
ATOM	2927	CA GLN	388	27. 024 80. 760	23. 030 23. 177	1.00 22.21 1.00 23.86	A	•
ATOM	2928	CG GLN	388	25. 745 80. 343	22. 477	1.00 23.80	A A	C C
ATOM	2929	CD GLN	388	25. 096 79. 126	23. 109	1.00 23.81	Ä	C
ATOM	2930	OE1 GLN	388	24. 357 78. 391	22. 452	1.00 34.98	Â	Õ
ATOM	2931	NE2 GLN	388	25. 356 78. 913	24. 395	1.00 34.36	A	N
ATOM	2932	C GLN	388	29. 403 80. 382	22. 427	1.00 21.72	Ä	C
ATOM	2933	0 GLN	388	29. 845 81. 428	22. 893	1.00 22.74	Ä	ŏ
ATOM	2934	N ILE	389	29. 982 79. 745	21.415	1.00 20.66	A	N
ATOM	2935	CA ILE	389	31. 231 80. 215	20. 821	1.00 21.00	Ä	Č
ATOM	2936	CB ILE	389	31.466 79.617	19. 422	1.00 20.76	Ä	č
ATOM	2937	CG2 ILE	389	31.410 78.100	19.496	1.00 19.50	Ā	Č
ATOM	2938	CG1 ILE	389	30.448 80.165	18. 429	1.00 19.48	A	Č
MOTA	2939	CD1 ILE	389	30. 813 79. 864	16. 992	1.00 19.12	A	С

(C									
					FIG. 4-61				
ATOM ATOM ATOM ATOM ATOM	2940 2941 2942 2943 2944	O N CA	ILE ILE ASP ASP ASP	389 389 390 390 390	31. 483 81. 713 20. 735 1. 00 23. 29 A 32. 640 82. 146 20. 776 1. 00 22. 48 A 30. 423 82. 505 20. 611 1. 00 24. 96 A 30. 584 83. 953 20. 533 1. 00 26. 49 A 29. 932 84. 508 19. 275 1. 00 29. 09 A	C O N C C			
ATOM ATOM ATOM ATOM ATOM	2945 2946 2947 2948 2949	0D1 0D2 C		390 390 390 390 390	28. 467 84. 215 19. 216 1. 00 30. 91 A 27. 754 84. 955 18. 517 1. 00 35. 45 A 28. 029 83. 236 19. 858 1. 00 33. 49 A 30. 005 84. 676 21. 738 1. 00 26. 43 A 29. 402 85. 735 21. 603 1. 00 26. 54	0 0 C			
ATOM ATOM ATOM ATOM	2950 2951 2952 2953	N CA CB CG	LYS LYS LYS LYS	391 391 391 391	30. 163 84. 078 22. 910 1. 00 27. 05 A 29. 707 84. 679 24. 150 1. 00 28. 81 A 28. 348 84. 128 24. 566 1. 00 28. 62 A 27. 203 84. 790 23. 824 1. 00 31. 00 A	N C C C			
ATOM ATOM ATOM ATOM ATOM	2954 2955 2956 2957 2958	CE NZ	LYS LYS LYS LYS LYS	391 391 391 391 391	25. 867 84. 228 24. 256 1. 00 34. 06 A 24. 733 84. 772 23. 413 1. 00 33. 69 A 23. 454 84. 073 23. 742 1. 00 36. 51 A 30. 772 84. 369 25. 183 1. 00 29. 11 A 31. 192 83. 223 25. 327 1. 00 29. 45 A	C N C O			
ATOM ATOM ATOM ATOM ATOM	2959 2960 2961 2962 2963	N CA CB CG	LYS LYS LYS LYS LYS	392 392 392 392 392	31. 219 85. 401 25. 888 1. 00 29. 66 A 32. 281 85. 248 26. 872 1. 00 30. 67 A 33. 069 86. 558 26. 985 1. 00 28. 28 A 33. 516 87. 119 25. 636 1. 00 27. 07 A 34. 330 86. 098 24. 852 1. 00 27. 55 A	C C C			
ATOM ATOM ATOM ATOM	2964 2965 2966 2967	CE NZ C O	LYS LYS LYS LYS	392 392 392 392	34. 643 86. 588 23. 449 1. 00 26. 02 A 35. 369 87. 872 23. 495 1. 00 25. 63 A 31. 824 84. 797 28. 248 1. 00 31. 24 A 32. 637 84. 679 29. 162 1. 00 32. 17 A	C N C O			
ATOM ATOM ATOM ATOM ATOM	2968 2969 2970 2971 2972	N CA CB CG OD1	ASP ASP ASP ASP ASP	393 393 393 393 393	30. 531 84. 548 28. 403 1. 00 31. 57 A 30. 015 84. 098 29. 690 1. 00 33. 64 A 29. 052 85. 134 30. 271 1. 00 36. 88 A 29. 734 86. 450 30. 567 1. 00 41. 66 A 30. 607 86. 475 31. 467 1. 00 43. 84 A	C C C			
ATOM ATOM ATOM ATOM ATOM	2973 2974 2975 2976 2977	OD2 C O N CA	ASP ASP ASP CYS CYS	393 393 393 394 394	29. 409 87. 455 29. 895 1. 00 44. 39 A 29. 309 82. 761 29. 546 1. 00 32. 46 A 28. 294 82. 666 28. 859 1. 00 32. 91 A 29. 841 81. 731 30. 198 1. 00 30. 05 A 29. 243 80. 410 30. 115 1. 00 28. 94 A	C O N			
ATOM ATOM ATOM ATOM ATOM	2978 2979 2980 2981 2982	C O CB SG	CYS CYS CYS CYS THR	394 394 394 394 395	28. 312 80. 116 31. 282 1. 00 27. 56 A 28. 262 80. 858 32. 258 1. 00 27. 11 A 30. 336 79. 338 30. 033 1. 00 31. 03 A 31. 401 79. 166 31. 504 1. 00 34. 42 A 27. 570 79. 023 31. 167 1. 00 25. 71 A	C O C S			
ATOM ATOM ATOM ATOM ATOM ATOM	2983 2984 2985 2986 2987 2988	N CA CB OG1 CG2 C	THR THR THR	395 395 395 395 395 395	26. 645 78. 608 32. 204 1. 00 25. 01 A 25. 208 78. 512 31. 647 1. 00 25. 50 A 24. 709 79. 833 31. 407 1. 00 28. 36 A 24. 289 77. 779 32. 620 1. 00 21. 52 A 27. 048 77. 251 32. 772 1. 00 24. 22 A 27. 196 76. 280 32. 036 1. 00 24. 44 A	C C O C			

										(Continued)
					FΙ	G. 4	- 62			(Oomminaca)
ATOM	2989	· N	PHE	396	27. 231	77. 185	34. 084	1.00 23.09	A	N
ATOM	2990	CA	PHE	396	27. 594	75. 924	34. 715	1.00 23.03	Ä	Ċ
ATOM	2991	CB	PHE	396	28. 138	76. 182	36. 116	1.00 22.19	A	Č
ATOM	2992	ĊĠ	PHE	396	29. 581	76.617	36. 131	1.00 23.20	A	Č
ATOM	2993		PHE	396	30.604	75.697	35. 876	1.00 22.48	Ä	Č
ATOM	2994		PHE	396	29. 924	77.935	36.415	1.00 20.97	Ā	Č
ATOM	2995		PHE	396	31.949	76.086	35. 908	1.00 20.26	Ä	Č
ATOM	2996		PHE	396	31. 267	78. 331	36. 447	1.00 21.70	. A	Č
ATOM	2997	CZ	PHE	396	32. 279	77.400	36. 194	1.00 20.27	A	Č
ATOM	2998	C	PHE	396	26.373	75.008	34.764	1.00 20.96	A	Č
ATOM	2999	0	PHE	396	25.311	75.412	35. 218	1.00 20.96	Ā	0
ATOM	3000	N	ILE	397	26.523	73.779	34.279	1.00 18.88	Ā	Ň
ATOM	3001	CA	ILE	397	25.412	72.842	34. 262	1.00 18.00	Α	C
ATOM	3002	CB	ILE	397	25.266	72.165	32.879	1.00 16.55	A	C
ATOM	3003	CG2	ILE	397	25.350	73. 209	31.787	1.00 13.63	A	Ċ
ATOM	3004	CG1	ILE	397	26.366	71.130	32.669	1.00 16.02	A	C
ATOM	3005	CD1	ILE	397	26.180	70.327	31.402	1.00 17.85	A	C
ATOM	3006	C	ILE	397	25. 527	71.770	35. 338	1.00 19.16	Α	С
ATOM	3007	0	ILE	397	24. 787	70.787	35.330	1.00 20.44	Α	0
ATOM	3008	N	THR	398	26.480	71.956	36. 244	1.00 18.55	Α	N
ATOM	3009	CA	THR	398	26.681	71.051	37. 367	1.00 19.41	Α	С
ATOM	3010	CB	THR	398	27. 624	69.858	37.051	1.00 19.56	Α	С
ATOM	3011		THR	398	28.978	70.321	36.960	1.00 22.60	Α	0
ATOM	3012	CG2	THR	398	27. 221	69.178	35.759	1.00 18.50	Α	С
ATOM	3013	C	THR	398	27. 343	71.899	38.424	1.00 20.24	Α	С
ATOM	3014	0	THR	398	27.979	72.903	38.104	1.00 20.11	Α	0
ATOM	3015	N	LYS	399	27.185	71.511	39.681	1.00 22.48	Α	N
ATOM	3016	CA	LYS	399	27. 795	72.258	40.772	1.00 23.72	A	С
ATOM	3017	CB	LYS	399	27. 111	73.618	40.941	1.00 24.42	Α	C ·
ATOM	3018	CG	LYS	399	25. 689	73. 583	41.462	1.00 27.65	Α	C
ATOM	3019	CD	LYS	399	25. 269	74.996	41.856	1.00 30.77	Α	С
ATOM	3020	CE	LYS	399	23.861	75.054	42.414	1.00 31.89	Α	C
ATOM	3021	NZ	LYS	399	22. 841	74. 747	41.377	1.00 35.03	Α	N ·
ATOM	3022	C	LYS	399	27. 751	71.476	42.077	1.00 22.46	Α	C
ATOM	3023	0	LYS	399	27. 125	70.425	42. 15 <u>4</u>	1.00 21.96	Α	0
ATOM	3024	N	GLY	400	28. 435	71.989	43.093	1.00 21.98	Α	N
ATOM	3025	CA	GLY	400	28. 463	71.319	44. 378	1.00 22.66	Α	C
ATOM	3026	C	GLY	400	29. 891	71.115	44.839	1.00 24.94	Α	С
ATOM	3027	0	GLY	400	30. 831	71.449	44. 118	1.00 26.10	Α	0
ATOM	3028	N	THR	401	30.064	70.566	46.036	1.00 25.34	Α	N
ATOM	3029	CA	THR	401	31.400	70. 335	46.560	1.00 26.41	Α	C
ATOM	3030	CB	THR	401	31.443	70. 541	48. 095	1.00 27.75	A	C
ATOM	3031	0G1		401	30.615	69. 567	48. 741	1.00 31.37	A	0
ATOM	3032	CG2		401	30. 924	71.927	48. 448	1.00 27.06	A	C
ATOM	3033	C	THR	401	31. 923	68. 945	46. 197	1.00 24.83	A	C
ATOM	3034	0	THR	401	32.027	68. 049	47.036	1.00 26.74	A	0
ATOM	3035	N	TRP	402	32. 229	68. 790	44. 915	1.00 22.03	A	N
ATOM	3036	CA	TRP	402	32. 781	67. 569	44. 340	1.00 18.83	A	C
ATOM	3037	CB	TRP	402	31.741	66.460	44.268	1.00 16.39	A	C

					(Continued)
				FIG. 4-63	
ATOM ATOM	3038 3039		402 402	30. 434 66. 886 43. 709 1. 00 17. 90 A 30. 037 66. 865 42. 332 1. 00 19. 16 A	C C
ATOM	3040		402	28. 701 67. 320 42. 278 1. 00 20. 21 A	C
ATOM	3041	CE3 TRP	402	30. 679 66. 505 41. 137 1. 00 18. 78 A	Č
ATOM	3042	CD1 TRP	402	29. 364 67. 345 44. 409 1. 00 17. 97 A	č
ATOM	3043	NE1 TRP	402	28. 318 67. 605 43. 562 1. 00 20. 57 A	N
ATOM	3044		402	27. 989 67. 425 41. 078 1. 00 18. 32 A	Ċ
ATOM	3045	CZ3 TRP	402	29.972 66.608 39.943 1.00 19.71 A	Č
ATOM	3046	CH2 TRP	402	28. 637 67. 064 39. 924 1. 00 18. 98 A	Ċ
ATOM	3047	C TRP	402	33. 208 67. 983 42. 944 1. 00 18. 09 A	С
ATOM	3048	0 TRP	402	32.956 69.117 42.540 1.00 18.12 A	0
ATOM	3049	N GLU	403	33.831 67.089 42.191 1.00 17.78 A	N
ATOM	3050	CA GLU	403	34. 284 67. 484 40. 866 1. 00 19. 48 A	C
ATOM	3051	CB GLU	403	35. 776 67. 805 40. 926 1. 00 20. 26 A	C
ATOM	3052	CG GLU	403	36. 122 68. 824 41. 983 1. 00 21. 69 A	Ç
ATOM	3053	CD GLU	403	37. 433 69. 522 41. 721 1. 00 23. 95 A	C
ATOM ATOM	3054 3055	OE1 GLU OE2 GLU	403	37. 506 70. 728 42. 020 1. 00 25. 27 A	0
ATOM	3056	C GLU	403 403	38. 384 68. 880 41. 223 1. 00 24. 57 A 34. 028 66. 516 39. 716 1. 00 19. 74 A	0
ATOM	3057	0 GLU	403		C
ATOM	3058	N VAL	404	00 050 00 000 00 000 000 000	0
ATOM	3059	CA VAL	404	33. 957 67. 073 38. 508 1. 00 18. 47 A 33. 760 66. 273 37. 305 1. 00 17. 63 A	N C
ATOM	3060	CB VAL	404	33. 070 67. 073 36. 165 1. 00 14. 78 A	C
ATOM	3061	CG1 VAL	404	32. 974 66. 210 34. 914 1. 00 11. 14 A	C
ATOM	3062	CG2 VAL	404	31. 683 67. 515 36. 595 1. 00 12. 13 A	č
ATOM	3063	C VAL	404	35. 153 65. 875 36. 836 1. 00 18. 38 A	č
ATOM	3064	0 VAL	404	35. 986 66. 732 36. 567 1. 00 20. 01 A	ŏ
ATOM	3065	N ILE	405	35. 410 64. 579 36. 764 1. 00 18. 83 A	N
ATOM	3066	CA ILE	405	36.707 64.088 36.323 1.00 20.05 A	C
ATOM	3067	CB ILE	405	36. 868 62. 593 36. 653 1. 00 21. 78 A	C
ATOM	3068	CG2 ILE	405	38. 254 62. 123 36. 283 1. 00 16. 28 A	C
ATOM	3069	CG1 ILE	405	36. 591 62. 364 38. 146 1. 00 24. 51 A	C
ATOM	3070	CD1 ILE	405	37. 438 63. 218 39. 079 1. 00 26. 24 A	С
ATOM ATOM	3071 3072	C ILE	405	36. 858 64. 290 34. 817 1. 00 19. 94 A	C
ATOM	3072	O ILE N GLY	405	37. 912 64. 710 34. 345 1. 00 20. 67 A	0
ATOM	3074	CA GLY	406 406	35. 803 63. 990 34. 064 1. 00 19. 40 A 35. 869 64. 171 32. 627 1. 00 16. 85 A	N
ATOM	3075	CA GL1	406	04 500 00 000 04 004 4 00 40	C
ATOM	3076	0 GLY	406	00 450 40 040 40 040	C
ATOM	3077	N ILE	407	0.4 480 0.4 080 00 800	0 N
ATOM	3078	CA ILE	407	00 000 01 500 00 000	N C
ATOM	3079	CB ILE	407	33. 303 64. 569 29. 852 1. 00 16. 98 A 33. 173 65. 861 28. 998 1. 00 16. 67 A	C C
ATOM	3080	CG2 ILE	407	32. 157 65. 671 27. 874 1. 00 16. 93 A	C
ATOM	3081	CG1 ILE	407	32. 779 67. 036 29. 895 1. 00 16. 45 A	Č
ATOM	3082	CD1 ILE	407	32. 646 68. 357 29. 157 1. 00 11. 65 A	č
ATOM	3083	C ILE	407	33.611 63.392 28.934 1.00 18.17 A	č
ATOM	3084	0 ILE	407	34. 599 63. 421 28. 212 1. 00 18. 89 A	Ŏ
ATOM	3085	N GLU	408	32. 766 62. 367 28. 945 1. 00 20. 84 A	N
ATOM	3086	CA GLU	408	33. 000 61. 176 28. 122 1. 00 22. 31 A	С

		٠.		EIC 4-64		(Continued)
				FIG. 4-64		
ATOM	3087	CB GLU	408	32. 691 59. 922 28. 944 1. 00 21. 64	A	C
ATOM	3088	CG GLU	408	33. 457 59. 860 30. 254 1. 00 23. 48 34. 963 59. 947 30. 048 1. 00 26. 15	A A	C C
ATOM ATOM	3089 3090	CD GLU OE1 GLU	408 408	35. 519 59. 081 29. 337 1. 00 28. 40	A	ŏ
ATOM	3090	OE2 GLU	408	35.594 60.877 30.596 1.00 25.87	Ä	Ö
ATOM	3092	C GLU	408	32.262 61.097 26.780 1.00 22.35	A	Ċ
ATOM	3093	0 GLU	408	32.743 60.455 25.846 1.00 23.83	A	0
ATOM	3094	N ALA	409	31.100 61.729 26.671 1.00 22.21	A	N
ATOM	3095	CA ALA	409	30. 356 61. 685 25. 414 1. 00 20. 74	A	C
ATOM	3096	CB ALA	409	29. 797 60. 294 25. 180 1. 00 21. 17	A	C
ATOM	3097	C ALA	409	29. 235 62. 708 25. 386 1. 00 20. 05	A	C
ATOM	3098	0 ALA	409	28. 651 63. 041 26. 413 1. 00 19. 39	A	O N
MOTA	3099	N LEU	410	28. 937 · 63. 201 · 24. 195 · 1. 00 · 19. 25 27. 911 · 64. 207 · 24. 038 · 1. 00 · 19. 28	A A	C
ATOM ATOM	3100 3101	CA LEU CB LEU	410 410	28. 559 65. 571 23. 796 1. 00 19. 29	A	Č
ATOM	3102	CG LEU	410	27. 634 66. 778 23. 617 1. 00 20. 83	A	č
ATOM	3102	CD1 LEU	410	26. 959 67. 089 24. 935 1. 00 20. 92	A	Č
ATOM	3104	CD2 LEU	410	28. 434 67. 987 23. 134 1. 00 20. 28	Α	С
ATOM	3105	C LEU	410	26. 998 63. 874 22. 879 1. 00 20. 25	A	С
ATOM	3106	0 LEU	410	27. 453 63. 649 21. 758 1. 00 20. 84	A	0
ATOM	3107	N THR	411	25. 701 63. 834 23. 150 1. 00 19. 86	A	N ·
ATOM	3108	CA THR	411	24. 741 63. 561 22. 100 1. 00 18. 40	A	C
ATOM	3109	CB THR	411	23. 902 62. 339 22. 418 1. 00 15. 82	A	C
ATOM	3110	OG1 THR	411	23. 017 62. 649 23. 498 1. 00 15. 79 24. 797 61. 177 22. 811 1. 00 14. 12	A A	0 C
ATOM ATOM	3111 3112	CG2 THR C THR	411 411	24. 797 61. 177 22. 811 1. 00 14. 12 23. 846 64. 787 22. 050 1. 00 20. 16	A	C
ATOM	3113	0 THR	411	23. 971 65. 684 22. 882 1. 00 21. 79	A	ŏ
ATOM	3114	N SER	412	22.952 64.836 21.074 1.00 20.25	A	Ň
ATOM	3115	CA SER	412	22.061 65.972 20.945 1.00 21.09	Ā	Ĉ
ATOM	3116	CB SER	412	21. 206 65. 827 19. 687 1. 00 22. 27	A	C
ATOM	3117	OG SER	412	20.474 64.618 19.721 1.00 25.03	A	0
ATOM	3118	C SER	412	21.158 66.118 22.153 1.00 21.84	A	C
ATOM	3119	0 SER	412	20. 598 67. 185 22. 379 1. 00 22. 97	A	0
ATOM	3120	N ASP	413	21.015 65.054 22.934 1.00 22.56	A	N
ATOM	3121	CA ASP	413	20.138 65.104 24.097 1.00 24.36 19.036 64.047 23.975 1.00 26.84	A A	C C
ATOM	3122	CB ASP CG ASP	413 413	19. 036 64. 047 23. 975 1. 00 26. 84 18. 161 64. 243 22. 751 1. 00 30. 28	A	C
ATOM ATOM	3123 3124	CG ASP OD1 ASP	413	17. 153 63. 515 22. 635 1. 00 32. 47	A	Ö
ATOM	3125	OD2 ASP	413	18.474 65.111 21.904 1.00 31.81	Ä	ŏ
ATOM	3126	C ASP	413	20. 822 64. 918 25. 442 1. 00 24. 37	A	Č
ATOM	3127	0 ASP	413	20.306 65.363 26.470 1.00 25.08	Α	0
ATOM	3128	N TYR	414	21. 974 64. 259 25. 444 1. 00 24. 23	A	N
ATOM	3129	CA TYR	414	22. 672 63. 998 26. 694 1. 00 23. 03	A	Ç
ATOM	3130	CB TYR	414	22. 369 62. 572 27. 155 1. 00 23. 61	A	C
ATOM	3131	CG TYR	414	20. 925 62. 332 27. 520 1. 00 25. 79	A	C
ATOM	3132	CD1 TYR	414	20.402 62.822 28.714 1.00 26.31	A	C
ATOM	3133	CE1 TYR	414	19.071 62.621 29.052 1.00 26.99	Α Δ	C C
ATOM	3134	CD2 TYR	414	20. 074 61. 629 26. 666 1. 00 24. 67 18. 740 61. 424 26. 993 1. 00 25. 53	A A	C
ATOM	3135	CE2 TYR	414	18.740 61.424 26.993 1.00 25.53	11	U

												(Cont	inued)
					F	I G.	4	- 65				(0012)	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
									1 00	00 20	٨	C	
ATOM	3136	CZ	TYR	414	18. 24		923	28. 188 28. 531		28.30 31.69	A A	C 0	
ATOM	3137	OH	TYR	414	16. 92 24. 18		. 731 . 174	26. 639		22. 81	A	Č	
ATOM	3138	C 0	TYR TYR	414 414	24. 10		. 040	25. 582		22.74	Ä	ŏ	
ATOM ATOM	3139 3140		LEU	415	24. 74		. 469	27. 809		20.51	Ä	Ň	
ATOM	3141		LEU	415	26. 17		630	27. 996		18. 28	Ä	C	
ATOM	3142		LEU	415	26. 50		079	28. 358		16.58	A	C	
ATOM	3143		LEU	415	27. 94		. 406	28.745		14.79	Α	C	
ATOM	3144	CD1		415	28. 18		. 892	28.606	1.00	13.01	A	C	
ATOM	3145	CD2		415	28. 20		. 943	30.163		14.04	A	C	
ATOM	3146	С	LEU	415	26. 51		. 684	29. 149		18.57	A	C	
ATOM	3147	0	LEU	415	25. 92		. 763	30. 230		18.31	A	0	
ATOM	3148	N	TYR	416	27.44		. 769	28. 909		19.11	A	N	
ATOM	3149	CA	TYR	416	27.84		. 796	29. 924		19.69	A	C	
ATOM	3150	CB	TYR	416	27. 96		. 407	29.309		18.66	A	C	
ATOM	3151	CG	TYR	416	26.69		. 926	28.645		17. 78 16. 67	A A	C	
ATOM	3152	CDI		416	26. 29		. 438 . 971	27. 410 26. 786		18.58	A	C	
ATOM	3153		TYR TYR	416 416	. 25. 13 25. 90		. 944	29. 245		16. 22	A	č	
ATOM ATOM	3154 3155		TYR	416	24. 75		. 475	28. 636		16.35	A	Č	
ATOM	3156	CZ	TYR	416			. 986	27.406		18.54	Ä	Č	
ATOM	3157	OH	TYR	416	23. 25		. 489	26. 784		19.53	Ā	Ö	
ATOM	3158	C	TYR	416	29. 16		. 178	30.540		20.71	Α	С	
ATOM	3159	0	TYR	416	30. 11		. 499	29.822	1.00	22.92	Α	0	
ATOM	3160	N	TYR	417	29. 23		. 138	31.866		19.27	Α	N	
ATOM	3161	CA	TYR	417	30.47		. 506	32.544		19.08	A	C	
ATOM	3162	CB	TYR	417	30.40		. 981	32.970		18.38	A	C	
ATOM	3163	CG	TYR	417	29. 38		. 282	34.049		17.93	A	C	
ATOM	3164		TYR	417	29. 72		. 213	35. 399		15. 25	A	C	
ATOM	3165		TYR	417	28. 78		. 476	36. 391		13.14	A	C	
ATOM	3166	CE2	TYR TYR	417 417	28. 07 27. 12		. 622 . 885	33. 718 34. 710		17.72 15.27	A A	C C	
ATOM ATOM	3167 3168	CZ	TYR	417	27. 48		. 808	36. 040		14. 25	A	Č	
ATOM	3169	OH	TYR	417	26. 5		. 046	37. 020		14.06	A	ŏ	
ATOM	3170	C	TYR	417	30. 76		. 615	33. 747		18.77	A	Č	
ATOM	3171	ŏ	TYR	417	29. 91		. 853	34. 207		18.74	A	Ō	
ATOM	3172	Ň	ILE	418	31.99		. 706	34. 236		17.63	Α	N	
ATOM	3173	CA	ILE	418	32. 42		. 926	35.379		16.60	Α	С	
ATOM	3174	CB	ILE	418	33. 63		. 019	35.015		15.54	A	С	
ATOM	3175		ILE	418	34.48		. 737	36. 241		14. 33	A	C	
ATOM	3176		ILE	418	33. 10		. 729	34. 378		15. 75	Ą	C	
ATOM	3177		ILE		34. 18		767	33. 964		15.48	A	C	
ATOM	3178	C	ILE	418	32. 82		. 909	36. 453		18.54	A	C	
ATOM	3179	0	ILE	418	33. 5		875	36. 190		20.83	A	O N	
ATOM	3180	N CA	SER SER	419 410	32. 3!		. 671	37. 664 38. 764		19.59 20.34	A A	C	
ATOM ATOM	3181 3182	CA CB	SER	419 419	32. 6′ 31. 5′		. 556 . 526	38. 996		21.79	A	Č	
ATOM	3183	OG	SER	419	30. 4		. 843	39. 562		24. 33	A	ő	
ATOM	3184	C	SER	419	32. 8		. 732	40.013		20. 37	Ä	Č	
111 014	-101	-	~~		52. 0				_, _,			-	

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					FI	G. 4	- 66			
ATOM	3185	0	SER	419	32.783	60. 503	39. 988	1.00 20.32	Α	0
ATOM	3186	N	ASN	420	33.152	62.427	41.107	1.00 19.64	Α	N
ATOM	3187	CA	ASN	420	33.357	61.786	42.387	1.00 20.07	Α	C
ATOM	3188	CB	ASN	420	34.773	62.053	42.863	1.00 18.49	Α	C
ATOM	3189	CG	ASN	420	35.099	63. 518	42.872	1.00 20.69	A	C
ATOM	3190	0D1		420	34. 210	64. 358	42.741	1.00 21.49	A	0
ATOM	3191	ND2		420	36.376	63.844	43. 034	1.00 21.39	Ą	N
ATOM	3192	C	ASN	420	32.350	62.368	43. 379	1.00 20.90	A	C
ATOM	3193	0	ASN	420	32.677	62.610	44. 535	1.00 21.17	A	0
ATOM	3194	N	GLU	421	31.127	62.600	42.914	1.00 21.68	A	N
ATOM	3195	CA	GLU	421	30.081	63. 160	43. 761	1.00 24.26	A	C C
ATOM	3196	CB	GLU	421	28. 935	63. 722	42.901	1.00 26.18	A	C
ATOM	3197	CG	GLU	421	27.714	64. 214 64. 817	43. 701 42. 824	1.00 25.32 1.00 26.09	A A	C
ATOM	3198	CD	GLU	421	26.604 25.563	65. 237	43. 373	1.00 20.09	A	Ö
ATOM	3199 3200	0E1	GLU	421 421	26.762	64. 873	41.588	1.00 27.22	A	Ö
ATOM ATOM	3200	C	GLU	421	29. 512	62. 133	44. 729	1.00 24.93	A	č
ATOM	3202	0	GLU	421	29.185	62. 457	45. 868	1.00 27.30	Ä	ŏ
ATOM	3203	N	TYR	422	29.409	60. 892	44. 272	1.00 23.63	Ä	Ň
ATOM	3204	CA	TYR	422	28. 837	59.826	45.075	1.00 23.67	A	Ċ
ATOM	3205	CB	TYR	422	28. 942	58. 503	44.311	1.00 23.61	Ā	Č
ATOM	3206	CG	TYR	422	28.015	57.415	44.813	1.00 24.39	Α	C
ATOM	3207		TYR	422	26.642	57.637	44.936	1.00 23.87	Α	C
ATOM	3208		TYR	422	25.781	56.618	45.347	1.00 22.11	Α	C
ATOM	3209	CD2	TYR	422	28.505	56.147	45.120	1.00 24.53	Α	С
ATOM	3210	CE2	TYR	422	27.654	55. 124	45. 533	1.00 23.32	Α	C
ATOM	3211	CZ	TYR	422	26.300	55. 367	45.641	1.00 23.52	A	Ç
ATOM	3212	OH	TYR	422	25. 471	54. 349	46.031	1.00 24.33	A	0
ATOM	3213	C	TYR	422	29. 399	59.679	46.493	1.00 23.57	A	C
ATOM	3214	0	TYR	422	30. 599	59. 478	46.704	1.00 23.17	A	0
ATOM	3215	N	LYS	423	28. 492	59. 784	47. 461	1.00 23.07	A	N
ATOM	3216	CA	LYS	423	28.813	59. 661	48. 878	1.00 22.04	A	C
ATOM	3217	CB	LYS	423	29. 156 27. 967	58. 205 57. 266	49. 205 49. 009	1.00 24.22 1.00 25.11	A A	C C
ATOM ATOM	3218 3219	CG CD	LYS LYS	$\begin{array}{c} 423 \\ 423 \end{array}$	28. 303	55. 809	49. 276	1.00 26.55	A	C
	3220		LYS	423	27.079	54. 930		1.00 28.11	A	C
ATOM ATOM	3221	NZ	LYS	423	27. 302	53. 498	49. 336	1.00 27.79	A	Ň
ATOM	3222	C	LYS	423	29. 923	60. 583	49. 347	1.00 21.46	Ä	Ċ
ATOM	3223	ŏ	LYS	423	30. 533	60. 340	50. 385	1.00 20.97	A	ŏ
ATOM	3224	Ň	GLY	424	30.167	61.647	48. 583	1.00 21.39	A	N
ATOM	3225	CA	GLY	424	31. 201	62.608	48. 930	1.00 21.20	A	Č
ATOM	3226	C	GLY	424		62.034	48.961	1.00 21.98	Α	C
ATOM	3227	Ö	GLY	424		62.534	49.687	1.00 22.19	Α	0
ATOM	3228	Ň	MET	425	32.848	60. 991	48.173	1.00 22.44	Α	N
ATOM	3229	CA	MET	425	34.161	60.350	48. 134	1.00 23.29	Α	C
ATOM	3230	CB	MET	425	34.003	58.826	48.056	1.00 24.14	Α	C
ATOM	3231	CG	MET	425	33. 548	58. 187	49. 360	1.00 25.32	Α	C
ATOM	3232	SD	MET	425	33.092	56. 451	49.179	1.00 29.39	Ą	S
ATOM	3233	CE	MET	425	34.663	55. 611	49. 406	1.00 27.92	A	C

			(Continued)							
ATOM	3234		MET	425	35. 042	G. 4 60.827		1.00 22.06	A	С
ATOM	3235		MET	425	34.836			1.00 22.61	Α	0
ATOM	3236		PRO	426	36.045		47. 292		Α	N
ATOM	3237		PRO	426	36. 386			1.00 21.34	A	C
ATOM	3238		PRO	426	36. 951	62. 172	46. 262	1.00 20.07	A	C
ATOM ATOM	3239 3240		PRO PRO	426	37. 943			1.00 20.22	A	C
ATOM	3240 3241	C	PRO	426 426	37. 138 37. 636		48. 245 45. 532	1.00 19.61	A	C
ATOM	3242		PRO	426	37. 030 37. 920			1.00 20.63 1.00 23.99	A	C
ATOM	3243		GLY	427	37. 905		46. 252	1.00 23.99	A A	O N
ATOM	3244		GLY	427	38. 552			1.00 18.08	Ä	C
ATOM	3245	C	GLY	427	37. 601	57. 838	44. 941	1.00 18.93	A	Č
ATOM	3246		GLY	427	37. 965	56. 706	44.642	1.00 21.55	Ä	ő
ATOM	3247	N	GLY	428	36. 378	58. 285	44.684	1.00 18.22	Ä	N
ATOM	3248	CA	GLY	428	35.417	57.446	43.991	1.00 17.96	Ā	C
ATOM	3249	C	GLY	428	35. 208	57.970	42.583	1.00 18.15	A	С
ATOM	3250	0	GLY	428	35. 577	59. 108	42.289	1.00 19.00	Α	0
ATOM	3251	N	ARG	429	34.619	57. 158	41.712	1.00 16.78	Α	N
ATOM	3252	CA	ARG	429	34. 389	57. 559	40. 320	1.00 17.38	Α	C
ATOM	3253	CB	ARG	429	35. 595	57. 167	39. 444	1.00 19.09	A	Č
ATOM ATOM	3254 3255	CG CD	ARG ARG	429	36. 577	58. 292	39. 108	1.00 20.57	A	C
ATOM	3256	NE	ARG	429 429	37. 385 38. 359	58. 737 59. 769	40.302	1.00 22.65	A	C
ATOM	3257	CZ	ARG	429	39. 078	60.445	39. 956 40. 852	1.00 25.75 1.00 26.83	A	N C
ATOM	3258		ARG	429	38. 927	60. 204	42. 146	1.00 26.78	A A	N N
ATOM	3259		ARG	429	39. 957	61.356	40. 456	1.00 26.16	A	N N
ATOM	3260	C	ARG	429	33. 134	56. 889	39.756	1.00 25.24	A	Č
ATOM	3261	0	ARG	429	32.976	55.675	39.857	1.00 12.14	Ä	ŏ
ATOM	3262	N	ASN	430	32. 256	57.679	39.146	1.00 14.98	Ä	Ň
ATOM	3263	CA	ASN	430	31.027	57.136	38. 586	1.00 17.41	Ā	Ċ
ATOM	3264	CB	ASN	430	29. 901	57. 216	39.622	1.00 17.29	A	C
ATOM	3265	CG	ASN	430	29. 947	56.081	40.620	1.00 18.53	Α	C .
ATOM	3266		ASN	430	29.607	54. 938	40. 297	1.00 16.68	Α	0
ATOM ATOM	3267 3268		ASN	430	30. 381	56. 386	41.840	1.00 15.65	A	N
ATOM	3269	C 0	ASN ASN	430	30. 564	57. 808	37. 297	1.00 17.98	A	C .
ATOM		N	LEU	430 431	30. 849 29. 840	00.9(0 57 059	31.U43	1.00 19.64	A	0
ATOM	3271	CA	LEU	431	29. 314	57. 053 57. 576	36. 485 35. 241	1.00 17.00	A	N
ATOM	3272	CB	LEU	431	29. 122	56. 442	34. 231	1.00 17.70 1.00 15.35	A	C
ATOM	3273		LEU	431	28. 478	56. 867	32. 913	1.00 15.33	A A	C
ATOM	3274		LEU	431	29. 340	57.917	32. 230	1.00 13.33	A A	C C
ATOM	3275		LEU	431	28. 296	55. 645	32.018	1.00 17.37	Ä	C
ATOM	3276	C	LEU	431	27. 978	58. 279	35. 491	1.00 19.03	A	Č
ATOM	3277	0	LEU	431	27. 095	57. 750	36. 172	1.00 17.62	A	ŏ
ATOM	3278	N	TYR	432	27.840		34. 933	1.00 20.33	Ä	N
ATOM	3279	CA	TYR	432	26.620	60. 248	35.083	1.00 21.23	Ä	Ċ
ATOM	3280	CB	TYR	432	26.848	61.442	36.014	1.00 22.85	Α	Ċ
ATOM	3281		TYR	432	27. 068	61.070	37.464	1.00 25.34	Α	C
ATOM	3282	CD1	TYR	432	28. 320	60. 646	37. 921	1.00 24.87	Α	C

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					ान	G. 4	- 6.8	•		(Continu	iea)
					1. 1	. 0. 1	0.0				
ATOM	3283	CR1	TYR	432	28. 519	60. 305	39. 267	1.00 24.97	Α	С	
ATOM	3284		TYR	432	26. 019			1.00 24.85	A	č	
ATOM	3285		TYR	432	26. 205			1.00 25.31	A	č	
ATOM	3286	CZ	TYR	432	27. 454			1.00 25.88	Ä	č	
ATOM	3287	OH	TYR	432	27. 629			1.00 25.59	A	Ŏ	
ATOM	3288	C	TYR	432	26. 102			1.00 21.26	A	č	
ATOM	3289	ŏ	TYR	432	26. 860			1.00 21.07	A	Ŏ	
ATOM	3290	N	LYS	433	24. 802			1.00 20.78	· A	Ň	
ATOM	3291	ĊA	LYS	433	24. 133			1.00 20.98	Â	Č	
ATOM	3292	CB	LYS	433	23. 290			1.00 21.14	Ä	č	
ATOM	3293	CG	LYS	433	22. 564			1.00 25.64	Ā	Č	
ATOM	3294	CD	LYS	433	21.843			1.00 25.30	A	Č	
ATOM	3295	CE	LYS	433	20.643			1.00 25.25	Ā	Č	
ATOM	3296	NZ	LYS	433	19. 801			1.00 27.99	A	Ň	
ATOM	3297	C	LYS	433	23. 228			1.00 20.46	A	Č	
ATOM	3298	Ŏ	LYS	433	22. 367			1.00 21.41	Ā	0	
ATOM	3299	N	ILE	434	23. 427			1.00 20.15	Α	N	
ATOM	3300	CA	ILE	434	22. 591			1.00 21.18	Α	C	
ATOM	3301	CB	ILE	434	23. 427			1.00 21.51	Α	C	
ATOM	3302		ILE	434	24. 412			1.00 22.39	Α	C	
ATOM	3303		ILE	434	22. 491			1.00 22.04	Α	C	
ATOM	3304		ILE	434	23. 171			1.00 23.38	Α	C	
ATOM	3305	C	ILE	434	21. 782			1.00 20.81	Α	C	
ATOM	3306	0	ILE	434	22. 274	65.154	30.056	1.00 21.15	Α	0	
ATOM	3307	N	GLN	435	20. 538			1.00 21.40	Α	N	
ATOM	3308	CA	GLN	435	19.666	66.034	30.248	1.00 23.73	Α	C	
ATOM	3309	CB	GLN	435	18. 202	65.851	30.646	1.00 26.08	Α	C	
ATOM	3310	CG	GLN	435	17. 227	66.030	29.496	1.00 29.99	Α	C	
ATOM	3311	CD	GLN	435	15. 802			1.00 32.10	Α	C	
ATOM	3312		GLN	435	15. 446			1.00 34.41	Α	0	
ATOM	3313	NE2	GLN	435	14. 978	66.839	29.819	1.00 34.05	Α	N	
ATOM	3314	C	GLN	435	19. 891			1.00 22.81	Α	C	
ATOM	3315	0	GLN	435	19.600			1.00 22.20	Α	0	
ATOM	3316	N	LEU	436	20. 401			1.00 23.57	A	N	
ATOM	3317	CA	LEU	436	20.679			1.00 24.55	Α	C	
ATOM	3318	CB	LEU	436	21. 152			1.00 21.18	Α	C	
ATOM	3319		LEU	436	22.456			1.00 21.36	Α	С	
ATOM	3320		LEU	436	22. 938			1.00 20.02	Α	C	
ATOM	3321		LEU	436	23. 510			1.00 19.70	Α	C	
ATOM	3322	C	LEU	436	19. 491			1.00 26.85	· A	C	
ATOM	3323	0	LEU	436	19.672			1.00 28.66	Α	0	
ATOM	3324	N	SER	437	18. 280			1.00 30.22	A	N	
ATOM	3325	CA	SER	437	17.059			1.00 32.38	A	C	
ATOM	3326	CB	SER	437	15. 925			1.00 32.98	A	C	
ATOM	3327	0G	SER	437	16. 241			1.00 39.22	A	0	
ATOM	3328	Ç	SER	437	16.610			1.00 33.81	A	C	
ATOM	3329	0	SER	437	15. 805			1.00 32.20	A	0	
ATOM	3330	N	ASP	438	17. 124			1.00 35.36	A	N	
ATOM	3331	CA	ASP	438	16.772	69.955	31. 784	1.00 36.00	Α	С	

					F I	G. 4	- 6 9			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3356 3357 3358 3359 3360 3361 3362 3363 3364 3365 3366 3367 3368	OD2 C O N CA CBC CD1 CE1 CC2 CC2 ON CA CBG CCD CC2 CC O N CA CBC CC O N CA CBC CC O N CA CBC CC O N CA CCB CC CC O N CA CCB CCC CC O N CA CCB CCC CC CCC CCC CCC CCC CCC CCC C	ASP ASP ASP ASP TYR TYR TYR TYR TYR TYR TYR TYR TYR TYR	438 438 438 438 439 439 439 439 439 439 439 439 439 440 440 440 440 441 441 441 441 441 441	15. 468 14. 996 15. 820 13. 796 17. 904 18. 019 18. 723 19. 862 20. 740 21. 262 21. 565 22. 071 21. 480 21. 987 22. 281 22. 803 19. 543 20. 435 18. 285 17. 917 16. 561 15. 507 16. 559 17. 794 17. 684 17. 808 17. 703 16. 871 15. 369 14. 848 13. 447 12. 953 19. 089 19. 668 19. 618 20. 922 21. 960	69. 226 69. 498 69. 415 69. 785 69. 470 68. 274 70. 412 70. 105 71. 343 71. 886 71. 028 71. 516 73. 253 73. 749 72. 875 73. 350 69. 624 69. 612 69. 67. 69. 624 69. 114 71. 144 67. 572 66. 829 67. 141 65. 735 65. 573 65. 490 66. 671 66. 392 67. 501 65. 119 65. 159 64. 564 63. 929 64. 717	32. 123 33. 543 34. 480 33. 725 32. 700 32. 993 33. 158 34. 013 34. 175 32. 867 31. 810 30. 611 32. 691 31. 496 30. 462 29. 284 35. 390 36. 076 37. 571 36. 953 37. 929 36. 780 37. 571 36. 953 37. 929 35. 697 35. 362 34. 088 34. 331 35. 122 35. 649 36. 243 37. 091	1. 00 41. 58 1. 00 43. 35 1. 00 43. 71 1. 00 35. 28 1. 00 33. 70 1. 00 34. 27 1. 00 33. 69 1. 00 32. 29 1. 00 30. 05 1. 00 28. 65 1. 00 28. 95 1. 00 27. 72 1. 00 28. 72 1. 00 33. 49 1. 00 34. 13 1. 00 34. 14 1. 00 33. 49 1. 00 32. 29 1. 00 30. 29 1. 00 30. 29 1. 00 30. 29 1. 00 30. 29 1. 00 30. 31 1. 00 32. 21 1. 00 30. 32 1. 00	A A A A A A A A A A A A A A A A A A A	CCOOCONCCCCCCCCOONCCCONCCCCNCONCC
ATOM ATOM ATOM	3369 3370	CG1 CG2	VAL	442 442 442 442	23. 266 22. 216 20. 786	63. 936 66. 084 62. 525	37. 178 36. 469 36. 807	1.00 24.82 1.00 22.99 1.00 23.65 1.00 24.10	A A	C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3372 (3373) 3374 (3375) 3376 (3377) 3378 (O N CA CB OG1 CG2 C	VAL THR THR THR THR	442 443 443 443 443 443 443 443 444	20. 327 21. 189 21. 109 20. 352 19. 017 20. 301 22. 493 23. 367 22. 701	62. 341 61. 539 60. 149 59. 306 59. 802 57. 862 59. 548 59. 792 58. 761	37. 931 36. 014 36. 419 35. 375 35. 222 35. 800 36. 551 35. 721 37. 596	1. 00 24. 10 1. 00 22. 60 1. 00 23. 16 1. 00 22. 78 1. 00 23. 02 1. 00 27. 68 1. 00 22. 12 1. 00 23. 54 1. 00 23. 36 1. 00 23. 18	A A A A A A A	C O N C C O C C C

					((Continued)
				FIG. 4-70		
ATOM	3381	CA CYS	444	23. 981 58. 104 37. 747 1. 00 24. 13 A		C
ATOM	3382	C CYS	444	23. 758 56. 712 37. 157 1. 00 22. 91 A		C
ATOM	3383	0 CYS	444	22. 855 55. 990 37. 573 1. 00 21. 72 A		0
ATOM	3384	CB CYS	444	24. 396 58. 018 39. 219 1. 00 25. 50 A		C
ATOM	3385	SG CYS	444	26. 053 57. 282 39. 443 1. 00 30. 81 A		S
ATOM	3386	n leu	445	24. 573 56. 348 36. 175 1. 00 22. 64 A		N
ATOM	3387	CA LEU	445	24. 446 55. 053 35. 513 1. 00 22. 51 A		C
ATOM	3388	CB LEU	445	24. 799 55. 211 34. 035 1. 00 19. 29 A		C
ATOM	3389	CG LEU	445	24. 049 56. 349 33. 341 1. 00 19. 36 A 24. 588 56. 552 31. 934 1. 00 16. 01 A		C
ATOM	3390	CD1 LEU	445			C
ATOM	3391	CD2 LEU	445			C
ATOM	3392	C LEU	445			Ö
ATOM	3393	0 LEU	445 446	25. 203 52. 783 35. 718 1. 00 24. 58 A 26. 148 54. 274 37. 087 1. 00 23. 95 A		N
ATOM	3394	N SER CA SER	446	27. 028 53. 269 37. 660 1. 00 23. 89 A		Ċ
ATOM ATOM	3395 3396	CB SER	446	28. 469 53. 555 37. 222 1. 00 21. 87 A		Č
ATOM	3397	OG SER	446	28. 882 54. 847 37. 648 1. 00 20. 09 A		0
ATOM	3398	C SER	446	26. 969 53. 145 39. 175 1. 00 23. 77 A		C
ATOM	3399	0 SER	446	27. 361 52. 119 39. 720 1. 00 24. 69 A	i	0
ATOM	3400	N CYS	447	26.480 54.184 39.845 1.00 24.32 A	i	N
ATOM	3401	CA CYS	447	26.382 54.207 41.309 1.00 26.45 A		С
ATOM	3402	C CYS	447	25.836 52.946 41.997 1.00 25.99		C
ATOM	3403	0 CYS	447	26. 441 52. 425 42. 937 1. 00 24. 44 A		0
ATOM	3404	CB CYS	447	25.518 55.396 41.763 1.00 27.33 A		C
ATOM	3405	SG CYS	447	26. 225 57. 049 41. 461 1. 00 34. 75		S
ATOM	3406	N GLU	448	24. 696 52. 456 41. 528 1. 00 25. 90 A		N C
ATOM	3407	CA GLU	448	24. 056 51. 317 42. 167 1. 00 24. 38 A 22. 581 51. 637 42. 334 1. 00 23. 47 A		C
ATOM	3408	CB GLU	448		4	C
ATOM	3409	CG GLU	448		À	č
ATOM	3410	CD GLU OE1 GLU	448 448		À	Ö
ATOM	3411	OE1 GLU	448		À	Ŏ
ATOM	3412 3413	C GLU	448		Ā	č
ATOM ATOM	3414	0 GLU	448		Ā	0
ATOM	3415	N LEU	449		A	N
ATOM	3416	CA LEU	449	25. 024 48. 547 39. 717 1. 00 23. 34	A	C
ATOM	3417	CB LEU	449	25. 988 48. 678 38. 548 1. 00 20. 76	A	C
ATOM	3418	CG LEU	449		A	C
ATOM	3419	CD1 LEU	449		A	C
ATOM	3420	CD2 LEU	449		A	C
ATOM	3421	C LEU	449		A	C
ATOM	3422	0 LEU	449		A	0 N
ATOM	3423	N ASN	450		A ^	N
ATOM	3424		450		A A	C
ATOM	3425	CB ASN	450		A A	C
ATOM	3426	CG ASN	450		A A	0
ATOM	3427	OD1 ASN	450 450		A	N
ATOM	3428 3429		450 450		A	Č
ATOM	3449	C WOIN	400	μι. υτι τι. τυι τυι του 1. ου 20. στ		•

F I G. 4 - 71										
ATOM ATOM ATOM ATOM	3430 3431 3432 3433	O AS N PI CD PI CA PI	RO 451 RO 451	29. 099 47. 637 43. 523 1. 00 26. 25 A 27. 210 48. 558 44. 303 1. 00 27. 04 A 25. 762 48. 411 44. 535 1. 00 27. 72 A	0 N C					
ATOM ATOM	3434 3435	CB PF	0 451 0 451	26. 579 49. 924 46. 103 1. 00 27. 21 A 25. 638 48. 765 45. 989 1. 00 25. 73 A	C C C					
ATOM ATOM ATOM	3436 3437 3438	C PF O PF N GI	kO 451 JU 452	28. 938 48. 983 46. 187 1. 00 28. 75 A 29. 877 49. 737 46. 433 1. 00 30. 69 A 28. 873 47. 746 46. 666 1. 00 29. 54 A	C O N					
ATOM ATOM ATOM ATOM	3439 3440 3441 3442	CA GI CB GI CG GI CD GI	.U 452 .U 452	29. 918	C C C					
ATOM ATOM ATOM	3443 3444 3445	OE1 GL OE2 GL C GL	.U 452 .U 452	27. 817 44. 848 49. 813 1. 00 45. 87 A 28. 084 43. 693 49. 402 1. 00 47. 97 A 27. 336 45. 076 50. 948 1. 00 47. 68 A 31. 221 46. 946 46. 816 1. 00 29. 63 A	C 0 0 C					
ATOM ATOM ATOM	3446 3447 3448	O GL N AR CA AR	U 452 G 453	32. 308 47. 199 47. 344 1. 00 30. 27 A 31. 099 46. 425 45. 600 1. 00 27. 01 A 32. 244 46. 057 44. 783 1. 00 24. 90 A	O N C					
ATOM ATOM ATOM	3449 3450 3451	CB AR CG AR CD AR	G 453 G 453	31. 950 44. 728 44. 085 1. 00 23. 08 A 32. 952 44. 337 43. 018 1. 00 22. 92 A 32. 602 42. 995 42. 381 1. 00 20. 49 A	C C C					
ATOM ATOM ATOM	3452 3453 3454	NE AR CZ AR NH1 AR	G 453 G 453	33. 504 42. 688 41. 278 1. 00 18. 31 A 33. 439 41. 595 40. 531 1. 00 18. 93 A 32. 510 40. 679 40. 763 1. 00 19. 77 A	N C N					
MOTA MOTA MOTA	3455 3456 3457	NH2 AR C AR O AR	G 453 G 453	34. 302 41. 425 39. 539 1. 00 18. 87 A 32. 695 47. 071 43. 738 1. 00 25. 72 A 33. 809 46. 962 43. 222 1. 00 24. 32 A	N C O					
ATOM ATOM ATOM ATOM	3458 3459 3460 3461	N CY CA CY C CY O CY	S 454 S 454	31. 857 48. 054 43. 420 1. 00 25. 94 A 32. 233 49. 012 42. 385 1. 00 25. 49 A 32. 038 50. 473 42. 699 1. 00 24. 24 A	N C C					
ATOM ATOM ATOM	3462 3463 3464	O CY CB CY SG CY N GL	S 454 S 454	30. 922 50. 970 42. 688 1. 00 26. 79 A 31. 503 48. 664 41. 096 1. 00 26. 13 A 32. 156 47. 128 40. 401 1. 00 30. 12 A 33. 143 51. 165 42. 942 1. 00 22. 97 A	0 C S					
ATOM ATOM ATOM	3465 3466 3467	CA GLI CB GLI CG GLI	N 455 N 455	33. 143 51. 165 42. 942 1. 00 22. 97 A 33. 105 52. 576 43. 276 1. 00 23. 69 A 33. 536 52. 761 44. 736 1. 00 23. 41 A 32. 564 52. 187 45. 761 1. 00 24. 96 A	N C C C					
ATOM ATOM ATOM	3468 3469 3470	CD GLI OE1 GLI NE2 GLI	N 455 N 455	33. 177 52. 065 47. 150 1. 00 29. 34 A 33. 981 52. 907 47. 574 1. 00 30. 98 A 32. 790 51. 022 47. 872 1. 00 28. 59 A	C O N					
ATOM ATOM ATOM	3471 3472 3473	C GLI O GLI N TYI	N 455 N 455 R 456	33. 992 53. 425 42. 360 1. 00 24. 57 A 33. 837 54. 645 42. 294 1. 00 27. 40 A 34. 919 52. 787 41. 654 1. 00 22. 57 A	C O N					
ATOM ATOM ATOM	3474 3475 3476	CA TYI CB TYI CG TYI	R 456 R 456	35. 821 53. 510 40. 763 1. 00 21. 75 A 37. 270 53. 187 41. 124 1. 00 20. 47 A 38. 267 54. 282 40. 817 1. 00 21. 27 A	C C C					
ATOM ATOM	3477 3478	CD1 TYI		38. 659 55. 193 41. 808 1. 00 20. 27 A 39. 618 56. 165 41. 548 1. 00 18. 67 A	C C					

					FΙ	G. 4	- 72			(Continued
ATOM	3479		TYR	456	38. 858	54. 385	39. 552	1.00 19.29	Α	C
ATOM	3480	CE2	TYR	456	39.812	55.353	39. 284	1.00 16.18	Α	С
ATOM	3481	CZ	TYR	456	40. 190	56. 236	40. 283	1.00 18.92	Α	С
ATOM	3482	OH	TYR	456	41. 151	57. 183	40.023	1.00 19.64	Α	0
ATOM	3483	C	TYR	456	35. 536	53.061	39. 335	1.00 21.96	A	Č
ATOM	3484	0	TYR	456	35. 944	51.972	38. 931	1.00 22.39	Ą	0
ATOM	3485	N	TYR	457	34. 846	53.899	38. 567	1.00 22.09	Ą	N.
ATOM	3486	CA	TYR	457	34. 499	53. 540	37. 196	1.00 20.82	A	C
ATOM	3487	CB	TYR	457	33. 001	53. 717	36.956	1.00 17.91	A	C
ATOM	3488	CG	TYR	457	32. 147	52. 613	37. 512	1.00 15.58	A	C
ATOM	3489		TYR	457	31.644	52. 674	38. 811	1.00 13.21	A	C
ATOM	3490		TYR	457	30. 830	51.668	39. 311	1.00 12.43	A	C
ATOM	3491		TYR	457	31.819	51.512	36.727	1.00 16.86	A	C
ATOM	3492		TYR	457	31.008	50. 497	37. 219	1.00 15.29	A	C
ATOM	3493	CZ	TYR	457	30.518	50. 582	38. 507	1.00 14.49	A	C
ATOM	3494	OH	TYR	457	29. 728	49.568	38. 985	1.00 15.62	A	0 C
ATOM	3495	C	TYR	457	35. 232	54. 240	36.066 36.227	1.00 21.27	A	0
ATOM	3496	0 N	TYR SER	457 458	35. 842 35. 132	55. 293 53. 622	34. 901	1.00 23.18 1.00 21.68	A	N N
ATOM ATOM	3497 3498	N CA	SER	458	35. 739	54. 108		1.00 21.08	A A	C
ATOM	3499	CB	SER	458 458	37. 083	53. 429	33. 474	1.00 21.74	A	C
ATOM	3500	OG	SER	458		53. 569	32. 141	1.00 29.63	A	0
ATOM	3501	C	SER	458	34. 751	53.664	32. 621	1.00 21.73	A	C
ATOM	3502	Ö	SER	458	34. 072	52.652	32. 804	1.00 20.08	A	0
ATOM	3503	N	VAL	459	34. 665	54. 405	31.520	1.00 20.58	Ä	N N
ATOM	3504	CA	VAL	459	33. 722	54.061	30.468	1.00 19.99	Ä	Č
ATOM	3505	CB	VAL	459	32. 457	54. 949	30. 568	1.00 19.45	A	č
ATOM	3506		VAL	459	32. 816	56. 392	30. 308	1.00 19.10	Ä	č
ATOM	3507		VAL	459	31.397	54. 475	29. 595	1.00 20.30	A	č
ATOM	3508	C	VAL	459	34. 309	54. 161	29.059	1.00 19.99	Ä	č
ATOM	3509	Ō	VAL	459	35. 314	54. 835	28. 831	1.00 21.13	Ä	Ö
ATOM	3510	N	SER	460	33.667	53.472	28.122	1.00 18.73	A	N
ATOM	3511	CA	SER	460	34.083	53.456	26.728	1.00 16.25	Α	Ĉ
ATOM	3512	CB	SER	460	34.970	52.230	26.476	1.00 16.33	Α	Ċ
ATOM	3513	0G	SER	460	35. 476	52.194	25.151	1.00 15.85	Α	0
ATOM	3514	C	SER	460	32.809	53.377		1.00 15.70	Α	С
ATOM	3515	0	SER	460	32.156	52.342	25.841	1.00 14.81	Α	0
ATOM	3516	N	PHE	461	32.450	54. 475	25. 226	1.00 16.00	Α	N
ATOM	3517	CA	PHE	461	31.245	54. 512	24.398	1.00 16.27	Α	C
ATOM	3518	CB	PHE	461	30. 636	55.921	24.367	1.00 15.50	Α	C
ATOM	3519	CG	PHE	461	30.001	56. 351	25.660	1.00 15.11	Α	C
ATOM	3520		PHE	461	30. 779	56. 764	26. 735	1.00 14.16	Α	С
ATOM	3521		PHE	461	28.617	56.340	25.804	1.00 14.86	A	C
ATOM	3522		PHE	461	30.190	57. 158	27. 931	1.00 12.94	A	C
ATOM	3523		PHE	461	28. 021	56. 733	26.996	1.00 12.76	A	C
ATOM	3524	CZ	PHE	461	28. 811	57. 142	28.061	1.00 11.01	A	Ċ
ATOM	3525	C	PHE	461	31.551	54. 102	22.971	1.00 17.94	A	C
ATOM	3526	0	PHE	461	32.686	54. 234	22.514	1.00 17.07	A	0
ATOM	3527	N	SER	462	30. 532	53.612	22.269	1.00 19.22	A	N

					FIG	G. 4	- 73			(Continued)
ATOM ATOM ATOM ATOM ATOM	3528 3529 3530 3531 3532	CA CB OG C	SER SER SER SER SER	462 462 462 462 462		53. 212 52. 381 53. 145 54. 496 55. 581	20. 877 20. 399 20. 397 20. 058 20. 577	1.00 23.70 1.00 23.50 1.00 24.06 1.00 24.95 1.00 25.95	A A A A	C C O C
ATOM ATOM ATOM	3533 3534 3535	N CA CB	LYS LYS LYS	463 463 463	31. 153	54. 373 55. 536 55. 084	18. 784 17. 920 16. 484	1.00 27.50 1.00 31.80 1.00 33.43	A A A	N C C
ATOM ATOM ATOM	3536 3537 3538	CG CD CE	LYS LYS LYS	463 463 463	33. 047 33. 972	55. 199 54. 435 54. 724	16. 075 17. 007 16. 673	1. 00 35. 54 1. 00 36. 78 1. 00 39. 20	A A	C C
ATOM ATOM	3539 3540	NZ C	LYS LYS	463 463	36. 384 30. 226	54. 098 56. 602	17. 641 17. 934	1.00 40.26 1.00 33.39	A A A	C N C
ATOM ATOM ATOM	3541 3542 3543	O N CA	LYS GLU GLU	463 464 464	29. 015 27. 945	57. 745 56. 254 57. 247	17. 561 18. 354 18. 410	1. 00 36. 36 1. 00 33. 23 1. 00 34. 54	A A A	O N C
ATOM ATOM ATOM	3544 3545 3546	CB CC CD	GLU GLU GLU	464 464 464	27. 528 26. 578	57. 058 57. 366 56. 961	17. 256 15. 882 14. 772	1. 00 39. 82 1. 00 44. 96 1. 00 48. 72	A A A	C C C
ATOM ATOM ATOM	3547 3548 3549	0E2 C	GLU GLU	464 464 464	26. 967 27. 186	57. 480 56. 120 57. 202	14. 752 13. 926 19. 729	1.00 50.39 1.00 50.59 1.00 32.77	A A A	0 0 C
ATOM ATOM ATOM	3550 3551 3552	O N CA	GLU ALA ALA	464 465 465	27. 823 27. 241	57. 659 56. 636 56. 546	19. 814 20. 748 22. 081	1.00 32.03 1.00 31.17 1.00 29.63	A A A	O N C
ATOM ATOM ATOM	3553 3554 3555	CB C O	ALA ALA	465 465 465	26. 015 25. 176	57. 935 55. 645 55. 824	22. 577 22. 164 23. 042	1.00 28.36 1.00 29.47 1.00 28.66	A A A	C C O
ATOM ATOM ATOM	3556 3557 3558	N CA CB	LYS LYS LYS	466 466 466	24. 763 24. 585	54. 678 53. 772 53. 122	21. 259 21. 274 19. 899	1.00 28.89 1.00 28.97 1.00 30.98	A A A	N C C
ATOM ATOM ATOM	3559 3560 3561	CG CD CE	LYS LYS LYS	466 466 466	23. 045 21. 632	52. 509 52. 179 51. 757	19. 649 18. 171 17. 814	1.00 31.77 1.00 34.52 1.00 35.82	A A A	C C C
ATOM ATOM ATOM	3562 3563 3564		LYS LYS	466 466 466	24. 987 24. 040	50. 441 52. 704 52. 126	22.869	1.00 38.42 1.00 28.20 1.00 27.93	A A A	N C O
ATOM ATOM ATOM	3565 3566 3567	N CA CB	TYR TYR TYR	467 467 467	26. 599 26. 955	52. 446 51. 458 50. 119	22. 646 23. 654 23. 003	1.00 26.93 1.00 26.21 1.00 27.94	A A A	N C C
ATOM ATOM ATOM	3568 3569 3570	CG CD1 CE1	TYR	467 467 467	25. 550 4 24. 494	49. 502 49. 917 49. 373	22. 207 20. 903 20. 184	1. 00 30. 39 1. 00 29. 93 1. 00 31. 13	A A A	C C C
ATOM ATOM ATOM	3571 3572 3573	CD2 CE2 CZ	TYR TYR	467 467 467	23. 953 4 23. 698 4	48. 522 47. 975 48. 405	22. 768 22. 060 20. 770	1. 00 29. 73 1. 00 30. 29 1. 00 30. 97	A A A	C C C
ATOM ATOM ATOM	3574 3575 3576	C	TYR TYR TYR	467 467 467	27. 777		20. 079 24. 470 24. 064	1. 00 32. 01 1. 00 24. 00 1. 00 24. 63	· A · A A	0 C 0

		,		FΙ	G. 4	- 74			(Continued)
ATOM	3577	N TY	R 468	27.969	51.370	25. 641	1.00 23.06	A	N
ATOM	3578	CA TY		29.091	51.765	26.462	1.00 22.80	Α	С
ATOM	3579	CB TY		28. 801	53.043	27. 249	1.00 23.88	Α	С
ATOM	3580	CG TY		27. 588	53.011	28. 155	1.00 24.49	Α	С
ATOM	3581	CD1 TY			53. 214	27.646	1.00 23.81	Α	С
ATOM	3582	CE1 TY		25. 206	53.308	28.486	1.00 25.51	Α	C
ATOM	3583	CD2 TY		27. 734	52.883	29.537	1.00 26.39	A	C
ATOM	3584	CE2 TY		26.638	52.971	30.390	1.00 25.67	Α	С
ATOM	3585	CZ TY	R 468	25.380	53. 191	29.857	1.00 25.81	Α	С
ATOM	3586	OH TY	R 468	24. 304	53. 334	30. 695	1.00 25.95	Α	0 .
ATOM	3587	C TY	R 468	29. 501	50.675	27.411	1.00 21.32	Α	C
ATOM	3588	0 TY	TR 468	28. 672	50.059	28.070	1.00 22.73	A	0
ATOM	3589	N GI		30. 800	50. 43 1	27. 449	1.00 20.26	A	N
ATOM	3590	CA GI		31.368	49. 429	28.315	1.00 19.27	Α	C
ATOM	3591	CB GI		32.643	48. 864	27.695	1.00 20.12	Α	. C
ATOM	3592	CG GI		33.460	47.993	28.632	1.00 21.72	A	C
ATOM	3593	CD GI		34. 891	47.845	28. 169	1.00 23.85	A	C
ATOM	3594	OE1 GI		35.605	48.837	28.011	1.00 25.81	A	0
ATOM	3595	NE2 GI		35. 322	46.609	27. 948	1.00 23.84	A	N
ATOM	3596	C GI		31.712	50. 158	29. 589	1.00 19.50	A	C
ATOM	3597	0 GI		32. 331	51. 226	29. 549	1.00 19.63	A	0
ATOM	3598	N LE		31. 277	49.611	30. 716	1.00 19.27	A	N
ATOM	3599	CA LE		31.602	50. 203	32.002	1.00 20.27	A	C
ATOM	3600	CB LF		30. 410	50.136	32.961	1.00 20.14	A	C
ATOM	3601	CG LE		29.442	51. 323	32.929	1.00 21.50	A	C
ATOM	3602	CD1 LE		28. 373	51.132	33.996	1.00 19.33	A	C
ATOM	3603	CD2 LE		30. 200	52. 620	33. 184	1.00 19.44	A	C
ATOM	3604	C LE		32.768	49.380	32. 531	1.00 20.91	Ą	C
ATOM	3605	0 LE		32. 785	48. 152	32. 409	1.00 19.97	A	0
ATOM	3606	N AF		33. 753	50.050	33. 102	1.00 22.57	A	N
ATOM	3607	CA AF		34. 917	49.344	33.610	1.00 25.83 1.00 29.78	A	C
ATOM	3608	CB AF		36. 137 35. 927	49. 690 49. 386	32. 748 31. 261	1.00 29.78	A	C C
ATOM	3609	CG AF		37. 091	49. 871	30. 426	1.00 31.73	A	C
ATOM ATOM	3610 3611	NE AF		36. 939	51. 261	30. 420	1.00 35.14	A A	N N
ATOM	3612	CZ AF		37. 961	52.061	29. 723	1.00 35.30	A	Č
ATOM	3613	NH1 AF		39. 202	51.606	29. 830	1.00 37.87	A	N
ATOM	3614	NH2 AF		37. 747	53. 304	29. 321	1.00 36.33	A	N
ATOM	3615	C AF		35. 171	49.686	35.064	1.00 24.89	A	C
ATOM	3616	0 AF		35. 685	50. 750	35. 388	1.00 27.07	Ä	ŏ
ATOM	3617	N C		34. 794	48. 766	35. 935	1.00 24.59	A	N
ATOM	3618	CA CY		34. 948	48. 925	37. 373	1.00 25.55	Ä	Ĉ
ATOM	3619	C CY		36. 328	48. 418	37. 806	1.00 23.33	A	č .
ATOM	3620	0 CY		36. 738	47. 319	37. 433	1.00 22.34	A	ŏ
ATOM	3621	CB CY		33. 812	48. 150	38. 059	1.00 26.66	A	č
ATOM	3622	SG CY		34. 037	47.670	39. 797	1.00 33.06	Ä	Š
ATOM	3623	N SE		37. 049	49. 219	38. 583	1.00 22.51	A	N
ATOM	3624	CA SE		38. 377	48. 809	39. 022	1.00 23.17	Ā	Ĉ
ATOM	3625	CB SE		39. 446	49.724	38. 414	1.00 21.92	Ā	Č
			- · ·		•				

					मा (G. 4	- 75			(Continued)
ATOM ATOM	3626 3627	OG C	SER SER	473 473	39. 500 38. 557	50. 976 48. 754	39. 071 40. 536	1. 00 23. 39 1. 00 23. 29	A A	0 C
ATOM	3628	0	SER	473	39. 685	48.758	41.028	1.00 24.44	Α	0
ATOM ATOM	3629 3630	N CA	GLY GLY	474 474	37. 457 37. 573	48. 697 48. 627	41. 279 42. 724	1.00 23.29 1.00 23.91	A A	N C
ATOM	3631	Č	GLY	474	36. 330	49.075	43. 459	1.00 24.41	A	č
ATOM	3632	0	GLY	474	35. 434	49.658	42.849	1.00 25.28	A	0
ATOM ATOM	3633 3634	N CD	PRO PRO	475 475	36. 257 35. 174	48. 850 49. 389	44. 780 45. 623	1.00 24.58 1.00 25.74	A A	N · C
ATOM	3635	CA	PR0	475	37. 280	48. 206	45.609	1.00 24.00	A	č
ATOM	3636	CB	PRO	475	36. 887	48. 620	47.022	1.00 22.53	A	C
ATOM ATOM	3637 3638	CG C	PRO PRO	475 475	35. 419 37. 397	48. 692 46. 692	46. 945 45. 462	1.00 25.59 1.00 24.86	A A	C C
ATOM	3639	ŏ	PRO	475	38. 294	46. 081	46.044	1.00 26.60	A	ő
ATOM	3640	N	GLY	476	36. 502	46.085	44.691	1.00 24.35	A	N
ATOM ATOM	3641 3642	CA C	GLY GLY	476 476	$36.564 \\ 37.324$	44. 646 44. 316	44. 498 43. 227	1.00 23.50 1.00 24.87	A A	C C
ATOM	3643	Õ	GLY	476	37. 925	45. 198	42.613	1.00 24.65	A	0
ATOM	3644	N	LEU	477	37. 308	43.054	42.818	1.00 24.78	Α	N
ATOM ATOM	3645 3646	CA CB	LEU LEU	477 477	38. 003 37. 927	42. 681 41. 171	41.601 41.383	1.00 25.85 1.00 26.86	A	C
ATOM	3647	CG	LEU	477	38. 661	40. 296	41. 363	1.00 20.80	A A	C C
ATOM	3648	CD1	LEU	477	38. 626	38.851	41.943	1.00 27.65	Ä	C
ATOM ATOM	3649 3650	CD2 C	LEU LEU	477	40. 102	40.759	42. 556	1.00 27.87	A	C
ATOM	3651	0	LEU	477 477	37. 369 36. 160	43. 417 43. 663	40. 424 40. 405	1.00 27.45 1.00 27.68	A A	C 0
ATOM	3652	N	PR0	478	38. 183	43.792	39. 428	1.00 27.18	A	N
ATOM	3653	CD	PRO	478		43.637	39. 362	1.00 27.65	A	C
ATOM ATOM	3654 3655	CA CB	PRO PRO	478 478		44. 505 44. 569	38. 253 37. 351	1.00 25.83 1.00 27.68	A A	C C
ATOM	3656	CG	PRO	478	40.023	44. 676	38. 335	1.00 27.43	A	C
ATOM	3657	C	PRO	478		43.806	37. 591	1.00 24.68	Α	C
ATOM ATOM	3658 3659	O N	PRO LEU	478 479	36. 464 35. 561	42. 583 44. 600	37. 506 37. 116	1.00 23.74 1.00 24.02	A	0 N
ATOM	3660	CA	LEU	479		44.068	36. 465	1.00 24.02	A A	N C
ATOM	3661	CB	LEU	479	33.186	44. 151	37.420	1.00 21.62	Ä	č
ATOM ATOM	3662 3663	CG CD1	LEU	479		43. 702	36. 854	1.00 21.11	A	C
ATOM	3664	CD1		479 479		42. 245 43. 901	36. 430 37. 912	1.00 21.98 1.00 24.17	A A	C C
ATOM	3665	C	LEU	479	4.077	44. 857	35. 199	1.00 22.18	A	č
ATOM	- 3666	0	LEU	479		46.073	35. 244	1.00 22.27	A	0
ATOM ATOM	3667 3668	N CA	TYR TYR	480 480		44. 160 44. 801	34. 073 32. 790	1.00 22.51 1.00 22.76	A A	N C
ATOM	3669	CB	TYR	480		44. 353	31. 749	1.00 22.59	A	Č
ATOM	3670	CG	TYR	480	36. 123	44.657	32. 147	1.00 21.95	Α	C
ATOM ATOM	3671 3672	CD1 CE1		480 480		45. 885 46. 190	31.843 32.249	1.00 22.81 1.00 23.84	A A	C C
ATOM	3673	CD2		480		40. 190 43. 733	32. 870	1.00 23.04	A A	C
MOTA	3674	CE2	TYR	480		44.027	33. 286	1.00 23.52	A	C

					FΙ	G. 4	- 76			(Continued)
ATOM	3675	CZ	TYR	480	38. 722	45. 257	32. 971	1.00 24.29	A	С
ATOM	3676	0H	TYR	480	39.998	45.556	33. 379	1.00 26.37	A	0
ATOM	3677	С	TYR	480	32, 291	44. 422	32.326	1.00 23.22	A	C
ATOM	3678	0	TYR	480	31.964	43. 239	32. 243	1.00 23.21	Α	0
ATOM	3679	N	THR	481	31.472	45.425	32.017	1.00 23.50	Α	N
ATOM	3680	CA	THR	481	30. 101	45. 181	31.577	1.00 22.82	Α	C
ATOM	3681	CB	THR	481	29.097	45.513	32.702	1.00 22.81	Α	C
ATOM	3682	0G1		481	29. 190	46.905	33.024	1.00 23.28	Α	0
ATOM	3683		THR	481	29. 398	44. 699	33. 951	1.00 21.29	A	C
ATOM	3684	C	THR	481	29.740	46.015	30. 351	1.00 23.25	Α	С
ATOM	3685	0	THR	481	30. 298	47. 091	30. 136	1.00 24.47	A	0
ATOM	3686	N	LEU	482	28. 809	45. 512	29. 547	1.00 23.21	A	N .
ATOM	3687	CA	LEU	482	28. 368		28. 350	1.00 23.54	A	Č
ATOM	3688	CB	LEU	482	28. 310	45. 268	27. 155	1.00 22.93	A	C
ATOM	3689	CG	LEU	482	28. 216	45. 922	25. 773	1.00 23.14	A	C
ATOM	3690		LEU	482	29. 483	46. 721	25. 507	1.00 23.20	A	C
ATOM	3691		LEU	482	28. 043	44. 861	24.699	1.00 22.53	A	C
ATOM	3692	C	LEU LEU	482	26. 981	46.767	28.643	1.00 23.83	A	C
ATOM ATOM	3693 3694	O N	HIS	482 483	26. 254 26. 610	46. 207 47. 861	29. 458 27. 994	1.00 25.57 1.00 22.84	A	0 N
ATOM	3695	CA	HIS	483 483	25. 301	48. 459	28. 231	1.00 22.84	A	N C
ATOM	3696	CB	HIS	483	25. 420	49. 528	29. 321	1.00 22.45	A	C
ATOM	3697	CG	HIS	483	26. 003	49. 025	30. 604	1.00 22.10	A A	C C
ATOM	3698		HIS	483	27. 289	48. 904	31.012	1.00 25.98	A	C
ATOM	3699		HIS	483	25. 228	48. 567	31.648	1.00 25.15	A	N
ATOM	3700		HIS	483	26. 011	48. 189	32. 644	1.00 23.13	A	Č
ATOM	3701		HIS	483	27. 266	48. 382	32. 283	1.00 22.74	A	Ň
ATOM	3702	C	HIS	483	24. 764	49.097	26. 950	1.00 22.46	A	č
ATOM	3703	Ö	HIS	483	25. 507	49. 281	25. 987	1.00 24.72	A	ŏ
ATOM	3704	N	SER	484	23. 475	49.427	26. 932	1.00 20.23	Ä	Ň
ATOM	3705	CA	SER	484	22.890	50.078	25.768	1.00 19.27	Ä	Ċ
ATOM	3706	CB	SER	484	21.789	49. 216	25.164	1.00 19.99	A	Ċ
ATOM	3707	0G	SER	484	20. 721	49.057	26.068	1.00 26.06	Α	0
ATOM	3708	C	SER	484	22.335	51.427	26. 213	1.00 19.12	Α	C
ATOM	3709	0	SER	484	21.656	51.521	27. 232	1.00 19.17	A	0
ATOM	3710	N	SER	485	22.628	52.470	25. 445	1.00 19.29	Α	N
ATOM	3711	CA	SER	485	22. 198	53.823	25. 783	1.00 20.52	A	С
ATOM	3712	CB	SER	485	23. 025	54. 841	25.000	1.00 20.72	Α	C
ATOM	3713	0G	SER	485	24. 386	54. 769	25. 379	1.00 23.68	Α	0
ATOM	3714	C	SER	485	20. 727	54. 160	25.604	1.00 20.05	Α	C
ATOM	3715	0	SER	485	20. 208	55.040	26. 287	1.00 18.92	A	0
ATOM	3716	N	VAL	486	20.055	53. 477	24. 688	1.00 20.23	A	N
ATOM	3717	CA	VAL	486	18.653	53. 764	24. 444	1.00 19.23	A	C
ATOM	3718	CB	VAL	486	18.058	52.816	23. 380	1.00 19.24	A	C
ATOM	3719		VAL	486	18.099	51.383	23. 869	1.00 19.40	A	C
ATOM	3720 3721	CGZ	VAL	486	16.635	53. 223	23. 070	1.00 20.10	A	C
ATOM ATOM	3722	0	VAL VAL	486 486	17.817	53.655	25. 705	1.00 19.72	A	C
ATOM	3723	N	ASN	486 487	16.869	54.415	25. 887	1.00 20.98	A	0
VION	0120	11	UNII	401	18. 190	52.727	26. 581	1.00 20.80	A	N

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(Continued) FIG. 4-77 **ATOM** 3724 CA ASN 487 52.464 17.458 27.824 1.00 20.70 С **ATOM** 3725 CB ASN 487 16.587 51.229 27.620 1.00 18.89 C 3726 **ATOM** CG ASN 487 17.403 50.007 C 27.171 1.00 22.56 A **ATOM** 3727 OD1 ASN 487 16.853 48.948 1.00 24.29 26.864 0 A 18.722 **ATOM** 3728 ND2 ASN 487 50.158 27.132 1.00 20.73 N A ATOM 3729 C ASN 18.354 487 52.220 29.047 1.00 22.59 C A ATOM 3730 0 ASN 487 17.865 51.758 1.00 22.43 30.079 0 A ATOM 3731 N ASP 488 19.650 52.514 28.929 1.00 23.24 N Α 20. 606 20. 415 ASP ASP 52. 290 ATOM 3732 CA 488 30.015 1.00 23.32 C A **ATOM** 3733 CB 488 53.304 31.148 1.00 24.08 $_{\rm C}^{\rm C}$ A ATOM 3734 CG **ASP** 488 20.780 54.718 30.750 1.00 24.71 A ATOM 3735 OD1 ASP 488 21.933 54.956 30.345 1.00 25.68 0 A 19.907 **ATOM** 3736 OD2 ASP 488 55.601 30.862 1.00 26.77 0 A **ATOM** 3737 C ASP 488 20.488 50.883 30.608 1.00 24.38 C ATOM 3738 0 ASP 488 20.709 50.689 31.803 1.00 24.38 A 0 **ATOM** 3739 LYS N 489 20.127 49.902 29.791 1.00 24.63 A N 20.009 **ATOM** 3740 LYS CA 489 48.541 30.300 1.00 25.48 C A 3741 3742 ATOM LYS 18.837 CB 489 47.817 29.630 1.00 25.85 \mathbf{C} Α ATOM CG LYS 489 17.651 47.594 30.579 1.00 28.57 Č A 3743 **ATOM** 17.247 CD LYS 489 48.906 31.251 1.00 30.67 \mathbb{C} A **ATOM** 3744 CE LYS 489 16.346 48.695 32.453 1.00 29.68 C Α **ATOM** 3745 NZ LYS 489 16.283 49.944 33.278 1.00 30.13 A N **ATOM** 3746 C LYS 489 21.297 47.749 1.00 26.05 30.110 Α C 21. 997 21. 605 **ATOM** 3747 0 LYS 489 47.914 29.106 1.00 26.23 A 0 ATOM 3748 GLY N 490 46.894 31.084 1.00 25.12 A N ATOM 3749 CA GLY 490 22.812 46.094 31.019 1.00 23.91 A C ATOM 3750 C GLY 490 22.694 44.966 30:017 1.00 25.29 C A ATOM 3751 0 GLY 490 21.85544.082 30.172 1.00 27.16 0 ATOM 3752 N LEU 491 23.531 28.986 44.991 1.00 24.58 A N ATOM 3753 CA LEU 491 23.503 43.953 27.969 1.00 24.98 C A ATOM 24. 298 23. 809 3754 CB LEU 491 44.385 26.737 1.00 25.21 A CCCCCATOM 3755 CG LEU 491 45.621 25.980 1.00 25.03 A 3756 CD1 ATOM LEU 491 24.796 45.968 24.881 1.00 22.44 A ATOM 3757 CD2 LEU 491 22.430 45.356 25.403 1.00 25.37 A ATOM 3758 C LEU 491 24.081 42.649 28.505 1.00 25.59 Α **ATOM** 3759 0 LEU 491 23.541 41.579 28.250 1.00 27.45 A **ATOM** 3760 N ARG 492 25.179 42.732 29.246 1.00 24.68 A N **ATOM** 41.529 3761 CA ARG 492 25.798 29.780 1.00 24.07 A C **ATOM** 3762 CB **ARG** 492 26.045 40.524 28.648 1.00 24.82 Α **ATOM** 3763 CG ARG 492 27.159 40.919 27.666 1.00 26.62 A C ATOM 3764 CD ARG 492 27.105 40.081 26.387 1.00 26.76 A C **ATOM** 3765 NE ARG 40. 357 492 25.884 25.641 1.00 29.45 N ATOM 3766 CZ ARG 492 25.708 41.414 24.855 1.00 30.52 Α C ATOM 3767 NH1 ARG 492 42.297 24.692 26.684 1.00 31.57 A N **ATOM** 3768 NH2 ARG 41.610 492 24.540 24. 261 1.00 29.62 N **ATOM** 3769 C ARG 492 27.117 41.831 30.473 1.00 23.83 C **ATOM** 3770 0 ARG 492 27.602 42.958 30.438 1.00 22.78 A 0 **ATOM** 3771 N VAL 493 27.680 40.807 31.109 1.00 24.93 N A 3772 ATOM CA VAL 493 28.966 40.911 31.791 1.00 25.89 C

				T) I		7.0			(Continued)
				F 1	G. 4				
ATOM	3773		AL 493				1.00 25.39 1.00 25.63	A A	C C
ATOM ATOM	3774 3775	CG1 V.	AL 493 AL 493				1.00 25.05	A	Č
ATOM	3776		AL 493				1.00 26.55	Ä	č
ATOM	3777		AL 493				1.00 29.06	. A	0
ATOM	3778		EU 494				1.00 26.28	Α	N
ATOM	3779		EU 494				1.00 25.35	Α	С
MOTA	3780		EU 494				1.00 23.74	A	C
ATOM	3781		EU 494		42. 554		1.00 22.82	A	C
ATOM	3782	CD1 L					1.00 22.34	A	C .
ATOM	3783 3784	CD2 L	EU 494 EU 494				1.00 19.11 1.00 26.29	A A	C C
ATOM ATOM	3785		EU 494				1.00 20.23	A	ŏ
ATOM	3786		LU 495				1.00 24.94	A	N
ATOM	3787		LU 495		39. 859		1.00 24.93	Ä	Ċ
ATOM	3788		LU 495		40. 445		1.00 24.61	Α	С
ATOM	3789	CG G	LU 495	37. 153	39.938		1.00 27.02	Α	С
ATOM	3790		LU 495				1.00 29.02	A	C
ATOM	3791	OE1 G					1.00 29.22	A	0
ATOM	3792	OE2 G					1.00 30.56	A	0
ATOM	3793		LU 495				1.00 25.32	A	C
ATOM ATOM	3794 3795		LU 495 SP 496				1.00 24.97° 1.00 25.38	A A	O N
ATOM	3796		SP 496				1.00 23.38	A	C
ATOM	3797		SP 496				1.00 27.17	A	č
ATOM	3798		SP 496				1.00 27.71	A	č
ATOM	3799	OD1 A					1.00 30.85	Ā	Ō
ATOM	3800	OD2 A		33. 898	36.657	36.360	1.00 29.23	Α	0
ATOM	3801		SP 496				1.00 27.65	Α	С
ATOM	3802		SP 496				1.00 27.02	A	0
ATOM	3803		SN 497				1.00 27.52	A	N
ATOM	3804		SN 497				1.00 29.40	A	C
ATOM ATOM	3805 3806		SN 497 SN 497				1.00 28.73 1.00 29.26	A A	C C
ATOM	3807		ISN 497				1.00 23.20	A	ő
ATOM	3808	ND2 A					1.00 31.42	A	Ň
ATOM	3809		SN 497				1.00 30.77	Ä	Ĉ
ATOM	3810		SN 497				1.00 31.70	Α	0
ATOM	3811		ER 498				1.00 31.77	Α	N
ATOM	3812		ER 498				1.00 31.32	Α	С
ATOM	3813		ER 498				1.00 32.01	A	C
ATOM	3814		ER 498				1.00 35.01	A	0
ATOM	3815		ER 498				1.00 30.55	A	C
ATOM	3816 3817		ER 498				1.00 31.44 1.00 29.46	A A	0 N
ATOM ATOM	3818		LA 499 LA 499				1.00 29.40	A	N C
ATOM	3819		LA 499 LA 499				1.00 27.47	A	Č
ATOM	3820		LA 499				1.00 30.28	A	č
ATOM	3821		LA 499				1.00 30.98	Ä	ŏ
		- ••				•			

		(Continued)			
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3826 CD1 3827 CD2 3828 C 3829 O 3830 N 3831 CA 3832 CB 3833 CG 3834 OD1 3835 OD2 3836 C 3837 O 3838 N 3839 CA 3840 CB 3841 CG 3841 CG 3842 CD 3843 CE 3844 NZ 3845 C 3846 O 3847 N	LEU 500 LEU 500 LEU 500 ASP 501 ASP 501 ASP 501 ASP 501 ASP 501	41. 218 36. 502 42. 106 37. 312 43. 459 36. 635 42. 269 38. 711 40. 251 35. 096	39. 223	(Continued) A N A C A C A C A C A C A C A C A C A C A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3849 CB 3850 CG 3851 SD 3852 CE 3853 C 3854 O 3855 N 3856 CA 3857 CB 3858 CG 3859 CD1 3860 CD2 3861 C 3862 O 3863 N 3864 CA 3865 CB 3866 CG 3867 CD 3868 OE1 3869 NE2	MET 503 MET 503 MET 503 MET 503 MET 503 MET 503 MET 504 LEU 505 GLN 505 GLN 505 GLN 505 GLN 505	42. 260 31. 733 43. 256 32. 193 43. 267 31. 332 44. 396 32. 004 45. 957 31. 226 42. 551 32. 530 43. 059 31. 990 42. 215 33. 815 42. 412 34. 700 41. 914 36. 103 42. 960 37. 197 44. 111 36. 668 42. 277 38. 376 41. 727 34. 211 42. 056 34. 664 40. 774 33. 292 40. 053 32. 737 38. 911 31. 834 37. 767 32. 574 37. 091 33. 544 36. 320 33. 143 37. 390 34. 829 40. 981 31. 920	42. 444 1. 00 45. 35 41. 200 1. 00 48. 35 39. 952 1. 00 54. 36 40. 438 1. 00 52. 89 44. 807 1. 00 41. 81 45. 790 1. 00 40. 44 44. 779 1. 00 41. 12 45. 919 1. 00 42. 37	A C C C A C C C A C C C A C C C A C C C A C

ATOM 3920 CG LYS 512 42.252 50.043 50.621 1.00 21.12 A C ATOM 3921 CD LYS 512 42.688 50.249 49.125 1.00 21.07 A C ATOM 3922 CE LYS 512 42.689 51.688 48.792 1.00 19.46 A C ATOM 3923 NZ LYS 512 42.779 51.870 47.343 1.00 15.688 A N ATOM 3924 C LYS 512 41.095 49.109 53.105 1.00 24.25 A C ATOM 3925 0 LYS 512 39.905 48.958 52.846 1.00 23.45 A O ATOM 3926 N LYS 513 41.546 50.017 53.960 1.00 24.50 A N ATOM 3927 CA LYS 513 41.546 50.017 53.960 1.00 24.50 A N ATOM 3928 C LYS 513 40.661 50.941 54.647 1.00 25.28 A C ATOM 3929 CG LYS 513 40.061 50.941 54.647 1.00 25.28 A C ATOM 3929 CG LYS 513 40.020 52.025 56.914 1.00 27.55 A C ATOM 3930 CD LYS 513 38.764 51.577 56.954 1.00 33.11 A C ATOM 3931 CE LYS 513 38.564 51.577 56.954 1.00 33.11 A C ATOM 3931 CE LYS 513 36.503 51.943 57.960 1.00 38.12 A N ATOM 3932 C LYS 513 36.503 51.943 57.960 1.00 38.12 A N ATOM 3933 C LYS 513 36.503 51.943 57.960 1.00 38.12 A N ATOM 3934 O LYS 513 340.806 52.312 53.999 1.00 26.42 A C ATOM 3934 O LYS 513 340.806 52.312 53.999 1.00 26.42 A C ATOM 3935 C LEU 514 39.888 52.891 53.575 1.00 25.40 A N ATOM 3937 CB LEU 514 39.888 52.891 53.575 1.00 25.40 A N ATOM 3937 CB LEU 514 39.888 52.891 53.575 1.00 25.40 A N ATOM 3937 CB LEU 514 39.888 52.891 53.575 1.00 25.40 A N ATOM 3939 CD1 LEU 514 38.816 55.143 50.825 1.00 20.88 A C ATOM 3940 CD2 LEU 514 38.816 55.153 49.476 1.00 22.59 A C ATOM 3941 C LEU 514 38.812 55.151 53.788 1.00 22.59 A C ATOM 3941 C LEU 514 38.812 55.151 53.788 1.00 22.59 A C ATOM 3941 C LEU 514 38.812 55.151 53.788 1.00 22.59 A C ATOM 3941 C LEU 514 38.812 55.151 53.788 1.00 22.59 A C ATOM 3941 C LEU 514 38.815 55.151 53.788 1.00 22.59 A C ATOM 3941 C LEU 514 38.812 55.151 53.788 1.00 22.59 A C ATOM 3941 C LEU 514 38.812 55.151 50.00 22.59 A C ATOM 3941 C LEU 514 38.812 55.151 50.00 22.59 A C ATOM 3941 C LEU 514 38.812 55.151 50.00 22.59 A C ATOM 3941 C LEU 514 38.812 55.151 50.00 22.59 A C ATOM 3941 C LEU 514 38.812 55.151 50.00 22.73 A C ATOM 3940 CD 2.89 515 38.89 57.905 56.851 1.00 22.59 A C ATOM 3940 CD 2.89 515 38.89 57.905 56.8					FIG. 4-81	(Continued)
ATOM 3928 CB LYS 513	ATOM ATOM ATOM ATOM ATOM ATOM	3921 CI 3922 CE 3923 NZ 3924 C 3925 O 3926 N	D LYS E LYS Z LYS LYS LYS LYS	512 512 512 512 512 513	42. 252 50. 043 50. 621 1. 00 21. 12 A 42. 368 50. 249 49. 125 1. 00 21. 07 A 42. 639 51. 688 48. 792 1. 00 19. 46 A 42. 779 51. 870 47. 343 1. 00 15. 68 A 41. 095 49. 109 53. 105 1. 00 24. 25 A 39. 905 48. 958 52. 846 1. 00 23. 45 A 41. 546 50. 017 53. 960 1. 00 24. 50 A	C C N C O N
ATOM 3936 CA LEU 514 39.688 54.213 52.958 1.00 22.53 A C ATOM 3937 CB LEU 514 39.147 54.119 51.536 1.00 20.88 A C ATOM 3938 CG LEU 514 38.866 55.443 50.825 1.00 21.52 A C ATOM 3939 CD1 LEU 514 40.149 56.242 50.662 1.00 21.52 A C ATOM 3940 CD2 LEU 514 38.846 55.443 50.825 1.00 22.59 A C ATOM 3940 CD2 LEU 514 38.812 55.153 49.476 1.00 22.59 A C ATOM 3941 C LEU 514 38.812 55.151 53.788 1.00 22.73 A C ATOM 3942 O LEU 514 37.591 54.981 53.844 1.00 20.65 A O ATOM 3943 N ASP 515 39.435 56.132 54.437 1.00 23.05 A N ATOM 3944 CA ASP 515 38.693 57.076 55.268 1.00 25.43 A C ATOM 3945 CB ASP 515 38.693 57.076 55.268 1.00 25.43 A C ATOM 3946 CG ASP 515 37.419 57.142 57.458 1.00 30.82 A C ATOM 3947 OD1 ASP 515 37.419 57.142 57.458 1.00 30.82 A C ATOM 3949 C ASP 515 36.639 57.905 56.851 1.00 32.73 A O ATOM 3949 C ASP 515 36.639 57.905 56.851 1.00 32.89 A O ATOM 3949 C ASP 515 38.693 57.905 56.851 1.00 32.89 A O ATOM 3950 O ASP 515 36.639 57.905 56.851 1.00 27.23 A O ATOM 3951 N PHE 516 39.107 59.230 56.345 1.00 27.23 A O ATOM 3951 N PHE 516 39.107 59.230 56.345 1.00 27.53 A N ATOM 3952 CA PHE 516 39.107 59.230 56.345 1.00 28.80 A C ATOM 3953 CB PHE 516 37.160 62.115 57.583 1.00 28.80 A C ATOM 3955 CD1 PHE 516 37.160 62.115 57.583 1.00 28.80 A C ATOM 3956 CD2 PHE 516 36.297 61.242 55.532 1.00 30.94 A C ATOM 3957 CEI PHE 516 35.002 61.279 56.058 1.00 28.84 A C ATOM 3957 CEI PHE 516 35.002 61.279 56.058 1.00 29.88 A C ATOM 3957 CEI PHE 516 35.002 61.279 56.058 1.00 29.88 A C ATOM 3957 CEI PHE 516 35.002 61.279 56.058 1.00 29.88 A C ATOM 3957 CEI PHE 516 35.002 61.279 56.058 1.00 29.88 A C ATOM 3958 CE2 PHE 516 35.002 61.279 56.058 1.00 29.88 A C ATOM 3960 C PHE 516 39.444 60.450 58.811 1.00 28.58 A C ATOM 3960 C PHE 516 39.444 60.450 58.811 1.00 28.58 A C ATOM 3960 C PHE 516 39.444 60.450 58.811 1.00 28.58 A C ATOM 3960 C PHE 516 39.444 60.450 58.811 1.00 29.42 A O ATOM 3961 C PHE 516 39.444 60.450 58.811 1.00 29.42 A O ATOM 3962 N ILE 517 40.773 62.053 57.990 1.00 28.66 A C ATOM 3964 CB ILE 517 40.773 62.053 57.990 1.00 28.66 A	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3928 CI 3929 CO 3930 CI 3931 CI 3932 NZ 3933 C 3934 O	B LYS G LYS D LYS E LYS Z LYS LYS LYS LYS	513 513 513 513 513 513	41. 040 51. 041 56. 124 1. 00 26. 65 A 40. 202 52. 025 56. 914 1. 00 27. 55 A 38. 754 51. 577 56. 954 1. 00 33. 11 A 37. 901 52. 476 57. 844 1. 00 35. 12 A 36. 503 51. 943 57. 960 1. 00 38. 12 A 40. 806 52. 312 53. 999 1. 00 26. 42 A 41. 918 52. 829 53. 877 1. 00 28. 66 A	C C C N C O
ATOM 3944 CA ASP 515 38.693 57.076 55.268 1.00 25.43 A C ATOM 3945 CB ASP 515 38.581 56.535 56.693 1.00 27.35 A C ATOM 3946 CG ASP 515 37.419 57.142 57.458 1.00 30.82 A C ATOM 3947 OD1 ASP 515 37.278 56.851 58.668 1.00 32.73 A O ATOM 3948 OD2 ASP 515 36.639 57.905 56.851 1.00 32.89 A O ATOM 3949 C ASP 515 39.346 58.462 55.287 1.00 26.80 A C ATOM 3950 O ASP 515 40.054 58.835 54.357 1.00 27.23 A O ATOM 3951 N PHE 516 39.107 59.230 56.345 1.00 27.53 A N ATOM 3952 CA PHE 516 39.688 60.566 56.431 1.00 28.71 A C ATOM 3953 CB PHE 516 38.780 61.590 55.729 1.00 28.60 A C ATOM 3954 CG PHE 516 37.387 61.658 56.291 1.00 28.84 A C ATOM 3955 CD1 PHE 516 36.297 61.242 55.532 1.00 30.94 A C ATOM 3957 CE1 PHE 516 36.297 61.242 55.532 1.00 30.94 A C ATOM 3958 CE2 PHE 516 35.875 62.157 58.116 1.00 28.99 A C ATOM 3959 CZ PHE 516 34.795 61.279 56.058 1.00 29.88 A C ATOM 3950 CZ PHE 516 34.795 61.279 56.058 1.00 29.88 A C ATOM 3950 CZ PHE 516 34.795 61.279 56.058 1.00 29.88 A C ATOM 3950 CZ PHE 516 34.795 61.279 56.058 1.00 29.88 A C ATOM 3950 CZ PHE 516 35.002 61.279 56.058 1.00 29.88 A C ATOM 3950 CZ PHE 516 34.795 61.737 57.352 1.00 29.33 A C ATOM 3950 CZ PHE 516 34.795 61.279 56.058 1.00 29.88 A C ATOM 3960 C PHE 516 39.943 61.024 57.861 1.00 28.58 A C ATOM 3960 C PHE 516 39.943 61.024 57.861 1.00 28.58 A C ATOM 3960 C PHE 516 39.943 61.024 57.861 1.00 29.42 A O ATOM 3961 O PHE 516 39.414 60.450 58.811 1.00 29.42 A O ATOM 3961 O PHE 516 39.414 60.450 58.811 1.00 29.42 A O ATOM 3962 N ILE 517 40.773 62.053 57.990 1.00 26.80 A N ATOM 3963 CA ILE 517 40.773 62.053 57.990 1.00 26.80 A N ATOM 3964 CB ILE 517 42.580 62.410 59.686 1.00 27.666 A C	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3936 CA 3937 CI 3938 CC 3939 CI 3940 CI 3941 C 3942 O	A LEU B LEU G LEU D1 LEU D2 LEU LEU LEU	514 514 514 514 514 514	39. 688 54. 213 52. 958 1. 00 22. 53 A 39. 147 54. 119 51. 536 1. 00 20. 88 A 38. 866 55. 443 50. 825 1. 00 21. 52 A 40. 149 56. 242 50. 662 1. 00 20. 94 A 38. 244 55. 153 49. 476 1. 00 22. 59 A 38. 812 55. 151 53. 788 1. 00 22. 73 A 37. 591 54. 981 53. 844 1. 00 20. 65 A	C C C C C
ATOM 3952 CA PHE 516 39.688 60.566 56.431 1.00 28.71 A C ATOM 3953 CB PHE 516 38.780 61.590 55.729 1.00 28.60 A C ATOM 3954 CG PHE 516 37.387 61.658 56.291 1.00 28.84 A C ATOM 3955 CD1 PHE 516 37.160 62.115 57.583 1.00 29.59 A C ATOM 3956 CD2 PHE 516 36.297 61.242 55.532 1.00 30.94 A C ATOM 3957 CE1 PHE 516 35.875 62.157 58.116 1.00 28.99 A C ATOM 3958 CE2 PHE 516 35.002 61.279 56.058 1.00 29.88 A C ATOM 3959 CZ PHE 516 34.795 61.737 57.352 1.00 29.33 A C ATOM 3960 C PHE 516 39.943 61.024 57.861 1.00 28.58 A C ATOM 3961 O PHE 516 39.943 61.024 57.861 1.00 29.42 A O ATOM 3962 N ILE 517 40.773 62.053 57.990 1.00 26.80 A N ATOM 3963 CA ILE 517 41.094 62.651 59.272 1.00 28.68 A C ATOM 3964 CB ILE 517 42.580 62.410 59.686 1.00 27.66 A C	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3944 CA 3945 CI 3946 CC 3947 OI 3948 OI 3949 C 3950 O	A ASP B ASP G ASP D1 ASP D2 ASP ASP ASP	515 515 515 515 515 515 515	38. 693 57. 076 55. 268 1. 00 25. 43 A 38. 581 56. 535 56. 693 1. 00 27. 35 A 37. 419 57. 142 57. 458 1. 00 30. 82 A 37. 278 56. 851 58. 668 1. 00 32. 73 A 36. 639 57. 905 56. 851 1. 00 32. 89 A 39. 346 58. 462 55. 287 1. 00 26. 80 A 40. 054 58. 835 54. 357 1. 00 27. 23 A	C C O O C
ATOM 3959 CZ PHE 516 34.795 61.737 57.352 1.00 29.33 A C ATOM 3960 C PHE 516 39.943 61.024 57.861 1.00 28.58 A C ATOM 3961 O PHE 516 39.414 60.450 58.811 1.00 29.42 A O ATOM 3962 N ILE 517 40.773 62.053 57.990 1.00 26.80 A N ATOM 3963 CA ILE 517 41.094 62.651 59.272 1.00 28.68 A C ATOM 3964 CB ILE 517 42.580 62.410 59.686 1.00 27.66 A C	ATOM ATOM ATOM ATOM ATOM ATOM	3952 CA 3953 CI 3954 CO 3955 CI 3956 CI 3957 CI	A PHE B PHE G PHE D1 PHE D2 PHE E1 PHE	516 516 516 516 516 516	39. 688 60. 566 56. 431 1. 00 28. 71 A 38. 780 61. 590 55. 729 1. 00 28. 60 A 37. 387 61. 658 56. 291 1. 00 28. 84 A 37. 160 62. 115 57. 583 1. 00 29. 59 A 36. 297 61. 242 55. 532 1. 00 30. 94 A 35. 875 62. 157 58. 116 1. 00 28. 99 A	C C C C C
ATOM 3965 CG2 ILE 517 42.799 60.937 59.989 1.00 23.78 A C ATOM 3966 CG1 ILE 517 43.538 62.861 58.581 1.00 29.30 A C ATOM 3967 CD1 ILE 517 43.676 64.361 58.431 1.00 31.79 A C	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3960 C 3961 O 3962 N 3963 CA 3964 CI 3965 CC 3966 CC	PHE PHE ILE A ILE B ILE G2 ILE G1 ILE	516 516 517 517 517 517 517	39. 943 61. 024 57. 861 1. 00 28. 58 A 39. 414 60. 450 58. 811 1. 00 29. 42 A 40. 773 62. 053 57. 990 1. 00 26. 80 A 41. 094 62. 651 59. 272 1. 00 28. 68 A 42. 580 62. 410 59. 686 1. 00 27. 66 A 42. 799 60. 937 59. 989 1. 00 23. 78 A 43. 538 62. 861 58. 581 1. 00 29. 30 A	C C O N C C C C

							•		(Continued)
			F	ΊG.	4 -	8 2			(Commingou)
ATOM 39 ATOM 40 ATOM 4	980 CB 981 CG 982 CD1 983 CD2 984 C 985 O 986 N 987 CA 988 CB 999 OD1 991 ND2 992 C 999 CA 999 CB 999 CB 999 CB 999 CB 000 CB 00	ILE 55 IL	17	313 64 516 64 516 66 5177 66 503 68 571 65 535 65 515 67 583 67 583 67 583 67 584 67 700 73 584 72 587 74 587 74 587 74 588 73 588 73 588 74 589 77 789 78 789 789 78 789 78 7	. 577 . 899 . 313 . 683 . 125 . 765 . 972 . 2069 . 126 . 326 . 326 . 326 . 326 . 326 . 328 . 328	57. 898 60. 102 59. 924 60. 283 60. 283 60. 455 60. 455 60. 455 60. 455 60. 321 60.	1. 00 31. 70 1. 00 32. 28 1. 00 33. 51 1. 00 33. 41 1. 00 33. 38 1. 00 33. 38 1. 00 35. 00 1. 00 35. 82 1. 00 36. 74 1. 00 39. 19 1. 00 39. 31 1. 00 39. 31 1. 00 39. 31 1. 00 39. 59 1. 00 40. 26 1. 00 40. 93 1. 00 41. 70 1. 00 42. 46 1. 00 44. 27 1. 00 46. 04 1. 00 47. 21 1. 00 42. 18 1. 00 42. 18 1. 00 42. 18 1. 00 42. 18 1. 00 42. 18 1. 00 42. 18 1. 00 42. 18 1. 00 42. 18 1. 00 42. 18 1. 00 42. 18 1. 00 42. 18 1. 00 42. 18 1. 00 42. 18 1. 00 42. 18 1. 00 42. 18 1. 00 42. 18 1. 00 43. 91 1. 00 50. 91 1. 00 50. 91 1. 00 50. 91 1. 00 30. 63 1. 00 33. 48 1. 00 33. 39 1. 00 33. 48 1. 00 33. 39 1. 00 33. 48 1. 00 33. 63	A A A A A A A A A A A A A A A A A A A	(Continued) ONCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
ATOM 40 ATOM 40 ATOM 40 ATOM 40 ATOM 40 ATOM 40 ATOM 40 ATOM 40	005 CB 006 0G1 007 CG2 008 C 009 0 010 N 011 CA	THR 5 THR 5 THR 5 THR 5 THR 5 THR 5 LYS 5 LYS 5	322 40. 322 40. 322 40. 322 39. 322 40. 323 38. 323 38.	339 70 127 72 364 70 357 68 086 68 653 68 685 66	0. 816 2. 223 0. 171 3. 706 3. 152 3. 045 5. 597	55. 584 55. 431 54. 202 56. 482 57. 305 55. 573 55. 479	1. 00 38. 55 1. 00 40. 51 1. 00 39. 39 1. 00 34. 94 1. 00 33. 48 1. 00 33. 07 1. 00 30. 63	A A A A A	C C C O N C
ATOM 44	008 C 009 O 010 N 011 CA 012 CB 013 CG 014 CD	THR 5 THR 5 LYS 5 LYS 5 LYS 5 LYS 5 LYS 5 LYS 5	522 39. 522 40. 523 38. 523 38. 523 37. 523 36. 523 35.	357 68 086 68 653 68 685 66 357 66 882 64 473 64	3. 706 3. 152 3. 045 5. 597 5. 105 4. 770	56. 482 57. 305 55. 573 55. 479 54. 901 55. 440 54. 956	1. 00 34. 94 1. 00 33. 48 1. 00 33. 07 1. 00 30. 63 1. 00 31. 78 1. 00 34. 92 1. 00 37. 12	A A A A A	C O N
ATOM 4	015 CE 016 NZ 017 C	LYS 5	523 34. 523 33. 523 39.	111 65	5. 296 5. 191	55. 455 54. 873 54. 576	1. 00 40. 20 1. 00 43. 74 1. 00 28. 84	A A A	N C

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								-			(Continued)
					FIG	. 4	- 83				(0022022200
ATOM	4018	0	LYS	523	39.962 6	6. 661	53. 448	1 00	29. 90	Α	0
ATOM	4018		PHE	524		55. 329	55. 086		26. 11	Ä	Ň
ATOM	4019		PHE	524		34. 858	54. 334		23. 17	Ä	Ċ
ATOM	4021		PHE	524		55.407	54. 953		22. 95	Ä	Č
ATOM	4022		PHE	524		6.854	54. 636		21.35	Ä	Č
ATOM	4023	CD1		524		57. 242	53. 346		21.14	Ā	Č
ATOM	4024	CD2		524		37. 830	55.620		18.86	Α	С
ATOM	4025	CE1		524		38. 587	53.040		19.22	A	С
ATOM	4026	CE2		524		39.171	55.329	1.00	19.37	Α	C
ATOM	4027	CZ	PHE	524		39. 552	54.034	1.00	19.34	Α	С
ATOM	4028	С	PHE	524	41.872	33. 337	54. 328		23. 15	A	C
ATOM	4029	0	PHE	524		52.703	55. 356		22.01	A	0
ATOM	4030	N	TRP	525		32.758	53. 156		24.00	A	N
ATOM	4031	CA	TRP	525		31.309	53.000		23. 65	A	C
ATOM	4032	CB	TRP	525		30. 958	51.696		23. 74	A	C
ATOM	4033	CG	TRP	525		31.452	51.647		24. 69	A	C
ATOM	4034	CD2		525		60. 687	51.893		25. 25	A	C
ATOM	4035	CE2		525		51.572	51.800		26. 02	A	C
ATOM	4036	CE3		525		59. 339	52. 186		25. 53	A	C
ATOM	4037			525		52. 732	51.418		25. 58	A	C
ATOM	4038	NE1		525		52. 815	51.508		25. 32	A	N C
ATOM	4039	CZ2		525		51. 151 58. 919	51.990 52.374		25. 72 24. 54	A	C C
ATOM	4040	CZ3 CH2		525 525		59. 824	52. 276		24. 86	A	C
ATOM ATOM	4041 4042	Cnz	TRP	525 525		50. 566	53. 042		23. 39	A A	C
ATOM	4042	0	TRP	525		51. 127	52. 803		24. 19	A	ŏ
ATOM	4043	N	TYR	526		59. 280	53. 347		22.63	A	N
ATOM	4045	CA	TYR	526		58. 412	53. 410	1 00	22.38	A	Ĉ
ATOM	4046	CB	TYR	526		58. 546	54. 763		22.15	Ä	č
ATOM	4047	CG	TYR	526		57. 946	55. 929		24.08	A	č
ATOM	4048		TYR	526		56. 574	56. 178		23.01	Ä	Č .
ATOM	4049		TYR	526		56.017	57. 204		25.01	Ä	Č
ATOM	4050		TYR	526		58. 748	56.747		24.62	A	Č
ATOM	4051		TYR	526		58. 205	57.772	1.00	24.74	Α	С
ATOM	4052	CZ	TYR	526		56.840	57.997		25.67	A	C
ATOM	4053	OH	TYR	526		56. 303	59.003		25.43	A	0
ATOM	4054	C	TYR	526	43. 478	56. 990	53. 251	1.00	22.00	A	C
ATOM	4055	0	TYR	526	42. 294	56. 724	53.482	1.00	21.71	A	0
ATOM	4056	N	GLN	527		56.084	52.843		19.68	Α	N
ATOM	4057	CA	GLN	527		54. 697	52.707		20.14	Α	С
ATOM	4058	CB	GLN	527		54. 301	51.238		19.56	A	C
ATOM	4059	CG	GLN	527		54. 422	50.465		23.06	A	Ç
ATOM	4060	CD	GLN	527		53. 890	49.065		23.49	A	C
ATOM	4061	0E1	GLN	527		54. 222	48. 359		25. 79	A	0
ATOM	4062	NE2	GLN	527		53.066	48.648		22.35	A	N
ATOM	4063	Ç	GLN	527		53. 871	53. 389		20.67	A	C
MOTA	4064	0	GLN	527		54. 334	53. 563		19.72	A	0
ATOM	4065	N	MET	528		52. 659	53. 792		21.11	A	N C
ATOM	4066	CA	MET	528	45.610	51.771	54. 460	1.00	22. 32	A	U

				FIG. 4-84						
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4067 4068 4069 4070 4071 4072 4073 4074 4075 4076 4077 4078 4081 4082 4083 4084 4085 4086 4087 4088 4090 4091 .4092 4093 4096 4097 4098 4100 4101	CB MET CG MET SD MET CE MET C MET O MET O MET C MET O MET C MET O MET C MET O MET C MET O	528 528 528 528 529 529 529 529 529 529 529 530 530 530 530 530 531 531 531 531 532 532 532 532	FIG. 4 - 84 45. 372 51. 753 55. 967 1. 00 23. 57 45. 830 52. 971 56. 727 1. 00 23. 53 45. 605 52. 683 58. 492 1. 00 23. 56 46. 400 54. 107 59. 158 1. 00 21. 91 45. 482 50. 347 53. 974 1. 00 23. 25 44. 383 49. 790 53. 935 1. 00 24. 82 46. 605 49. 751 53. 600 1. 00 22. 51 46. 587 48. 363 53. 183 1. 00 21. 97 47. 644 48. 078 52. 116 1. 00 19. 54 47. 557 46. 635 51. 681 1. 00 19. 54 47. 454 49. 029 50. 927 1. 00 21. 01 46. 045 49. 038 50. 335 1. 00 19. 28 46. 937 47. 620 54. 465 1. 00 24. 02 48. 114 47. 505 54. 820 1. 00 25. 51 45. 911 47. 153 55. 175 1. 00 24. 47 46. 114 46. 443 56. 438 1. 00 24. 76 44. 915 46. 640 57. 370 1. 00 24. 08 44. 451 48. 052 57. 726 1. 00 24. 08 44. 451 48. 052 57. 726 1. 00 24. 92 43. 365 47. 928 58. 763 1. 00 24. 92 43. 365 47. 928 58. 763 1. 00 24. 58 45. 589 48. 896 58. 272 1. 00 25. 50 46. 337 44. 953 56. 241 1. 00 24. 39 45. 686 44. 319 55. 411 1. 00 24. 58 47. 272 44. 374 57. 003 1. 00 24. 58 48. 174 45. 045 57. 950 1. 00 24. 42 47. 578 42. 943 56. 913 1. 00 26. 79 48. 763 42. 784 57. 862 1. 00 26. 79 48. 763 42. 784 57. 862 1. 00 26. 79 48. 763 42. 784 57. 862 1. 00 26. 79 48. 763 42. 784 57. 862 1. 00 28. 05 45. 443 42. 562 57. 931 1. 00 31. 01 46. 417 40. 782 56. 964 1. 00 28. 42 47. 484 40. 062 56. 253 1. 00 28. 68 45. 783 38. 534 56. 745 1. 00 28. 68 46. 726 38. 912 55. 659 1. 00 28. 50 45. 113 39. 799 58. 814 1. 00 29. 80						
ATOM ATOM ATOM ATOM	4101 4102 4103 4104		532 532 533 533	46.051 40.006 59.579 1.00 31.52 43.894 39.501 59.242 1.00 31.29	<i>l</i> 0					
ATOM ATOM ATOM	4105 4106 4107	CB HIS CG HIS CD2 HIS	533 533 533	44. 278 38. 127 61. 225 1. 00 29. 82 4 44. 170 36. 936 60. 324 1. 00 29. 23 4 45. 114 36. 247 59. 641 1. 00 28. 40 4	A C A C					
ATOM ATOM ATOM ATOM	4108 4109 4110 4111	ND1 HIS CE1 HIS NE2 HIS C HIS	533 533 533 533	43. 174 35. 326 59. 197 1. 00 28. 67 44. 469 35. 251 58. 949 1. 00 28. 85 44. 101 40. 601 61. 445 1. 00 33. 77	A N A C A N A C					
ATOM ATOM ATOM ATOM	4112 4113 4114 4115	O HIS N PHE CA PHE CB PHE	533 534 534 534	44. 121 41. 758 60. 787 1. 00 35. 52 44. 578 42. 987 61. 427 1. 00 37. 29	A O A N A C A C					

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					E 1 (G. 4	- 95			(Continued)
					r I v	J. 4	00			
ATOM	4116	CG	PHE	534	44. 510	45. 523	61.235	1.00 35.46	Α	С
ATOM	4117		PHE	534	45.811	45. 956	61.475	1.00 35.65	Ā	Č
ATOM	4118		PHE	534	43. 455	46. 320	61.654	1.00 33.35	A	Č
ATOM	4119		PHE	534	46.056	47.167	62. 124	1.00 36.55	A	Č
ATOM	4120		PHE	534	43. 688	47. 530	62. 304	1.00 35.26	Ā	Č
ATOM	4121	CZ	PHE	534		47. 957	62. 541	1.00 35.35	A	Č
ATOM	4122	C	PHE	534	43. 920	43. 158	62. 790	1.00 38.07	Ä	Č
ATOM	4123	ŏ	PHE	534	42. 705	43.046	62. 911	1.00 38.83	A	Ö
ATOM	4124	Ň	ASP	535	44. 725	43. 435	63. 810	1.00 39.27	A	N
ATOM	4125	CA	ASP	535	44. 206	43.621	65.160	1.00 40.72	A	C
ATOM	4126	CB	ASP	535	44. 751	42.541	66.089	1.00 43.14	A	Ċ
ATOM	4127	ĊĠ	ASP	535	44. 102	42.571	67.460	1.00 46.19	A	C
ATOM	4128		ASP	535	43.704	43.668	67.912	1.00 46.58	Α	0
ATOM	4129		ASP	535	43.999	41.499	68.092	1.00 48.00	Α	0
ATOM	4130	C	ASP	535	44.614	44.985	65.699	1.00 40.91	Α	C
ATOM	4131	Ō	ASP	535	45.799	45. 270	65.837	1.00 40.57	Α	0
ATOM ·	4132	N	LYS	536	43.635	45.822	66.022	1.00 41.40	Α	N
ATOM	4133	CA	LYS	536	43. 936	47.148	66.539	1.00 42.56	· A	C
ATOM	4134	CB	LYS	536	42.675	48.018	66.572	1.00 44.69	Α	С
ATOM	4135	CG	LYS	536	42. 146	48.406	65.200	1.00 47.06	Α	C
ATOM	4136	CD	LYS	536	41.156	49.566	65.289	1.00 49.52	Α	C
ATOM	4137	CE	LYS	536	40.721	50.020	63.897	1.00 50.85	Α	C
ATOM	4138	NZ	LYS	536	39. 965	51.303	63.921	1.00 51.05	Α	N
ATOM	4139	C	LYS	536	44. 553	47.105	67.928	1.00 42.57	Α	C
ATOM	4140	0	LYS	536	44.896	48.147	68.486	1.00 42.20	Α	0
ATOM	4141	N	SER	537	44. 697	45.907	68.486	1.00 42.80	Α	N
ATOM	4142	CA	SER	537	45. 277	45.762	69.820	1.00 43.70	Α	C
ATOM	4143	CB	SER	537	44. 744	44. 499	70. 513	1.00 44.09	Α	С
ATOM	4144	0G	SER	537	45. 222	43.319	69.888	1.00 43.50	Α	0
ATOM	4145	C	SER	537	46. 796	45.696	69. 737	1.00 43.27	Α	C
ATOM	4146	0	SER	537	47. 498	46.061	70.682	1.00 44.98	Α	0
ATOM	4147	N	LYS	538	47. 295	45. 230	68. 598	1.00 41.93	Α	N
ATOM	4148	CA	LYS	538	48. 729	45.110	68.380	1.00 40.13	A	C
ATOM	4149	CB	LYS	538	49. 024	43.917	67.470	1.00 41.29	A	Ċ
ATOM	4150	CG	LYS	538	48. 521	42. 590	68.013	1.00 42.24	A	Ċ
ATOM	4151	CD	LYS	538	48. 834	41.446	67.073	1.00 41.97	A	C
ATOM	4152	CE	LYS	538	48. 317	40. 140	67.638	1.00 42.57	A	C
ATOM	4153	NZ	LYS	538	46.864	40. 231	67. 960	1.00 44.10	A	N
ATOM	4154	C	LYS	538	49. 280	46.372	67. 741	1.00 38.59	A	C
ATOM	4155	0	LYS	538	48. 526	47. 229	67. 283	1.00 38.17	A	0
ATOM	4156	N	·LYS	539	50. 601	46. 485	67. 725	1.00 36.92	A	N
ATOM	4157	CA	LYS	539	51. 263	47. 629	67.116	1.00 36.43	A	C
ATOM	4158	CB	LYS	539	52. 293	48. 225	68. 079	1.00 37.32	A	C
ATOM	4159	CG	LYS	539	51.693	48. 838	69.341	1.00 37.42	A	C
ATOM	4160	CD	LYS	539	50. 925	50.117	69.028	1.00 40.01	A	C
ATOM	4161	CE	LYS	539	50. 209	50.674	70. 258	1.00 41.64	A	C
ATOM	4162	NZ	LYS	539	51.121	51.014	71.389	1.00 43.98	A	N
ATOM	4163	C	LYS	539	51.943	47.110	65. 849	1.00 35.38	A	C 0
MOTA	4164	0	LYS	539	52.699	46. 137	65. 893	1.00 35.49	A	U

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	•			FIG. 4-86	(Oonumace
4 TO 14	41.CE	NI TVD	540	51.658 47.747 64.719 1.00 33.00 A	N
ATOM	4165	N TYR CA TYR	540 540	52. 229 47. 316 63. 452 1. 00 30. 12 A	C
ATOM	4166 4167	CB TYR	540	51, 131 47, 135 62, 397 1, 00 28, 99 A	C
ATOM ATOM	4168	CG TYR	540	50, 204 45, 968 62, 630 1, 00 29, 13 A	С
ATOM	4169	CD1 TYR	540	49 109 46 078 63 488 1 00 28 32 A	С
ATOM	4170	CE1 TYR	540	48. 254 45. 000 63. 699 1. 00 27. 13 A	C
ATOM	4171	CD2 TYR	540	50. 421 44. 748 61. 990 1. 00 27. 62 A	C
ATOM	4172	CE2 TYR	540	49.576 43.669 62.196 1.00 26.32 A	C
ATOM	4173	CZ TYR	540	48. 495 43. 800 63. 051 1. 00 27. 64 A	C
ATOM	4174	OH TYR	540	47. 661 42. 724 63. 260 1. 00 29. 67 A	0
ATOM	4175	C TYR	540	53. 242 48. 287 62. 890 1. 00 29. 33 A	C 0
ATOM	4176	0 TYR	540	53. 130 49. 492 63. 091 1. 00 31. 23 A 54. 270 47. 772 62. 199 1. 00 27. 71 A	N N
ATOM	4177	N PRO	541	01.2.0	C
ATOM	4178	CD PRO	541	01.11.	C
ATOM	4179	CA PRO	541		Č
ATOM	4180	CB PRO	541	56. 361 47. 794 61. 148 1. 00 26. 81 A 55. 662 46. 512 60. 867 1. 00 25. 92 A	Č ·
ATOM	4181	CG PRO	541 541	54. 463 49. 358 60. 500 1. 00 27. 83 A	č
ATOM	4182	C PRO O PRO	541	53. 579 48. 727 59. 912 1. 00 28. 03 A	0
ATOM	4183 4184	O PRO N LEU	542	54. 763 50. 613 60. 200 1. 00 27. 70 A	N
ATOM ATOM	4185	CA LEU	542	54.032 51.307 59.154 1.00 26.55 A	C
ATOM	4186	CB LEU	542	53, 220 52, 440 59, 791 1, 00 26, 11 A	C
ATOM	4187	CG LEU	542	52, 252 53, 292 58, 959 1, 00 28, 68 A	С
ATOM	4188	CD1 LEU	542	51.422 54.170 59.898 1.00 29.38 A	C
ATOM	4189	CD2 LEU	542	53. 017 54. 165 57. 979 1. 00 29. 52 A	
ATOM	4190	C LEU	542	54. 924 51. 855 58. 042 1. 00 26. 16 A	
ATOM	4191	O LEU	542	55. 943 52. 492 58. 303 1. 00 28. 00 A	
ATOM	4192	n leu	543	54.536 51.589 56.801 1.00 23.70 A	
ATOM	4193	CA LEU	543	55. 263 52. 097 55. 651 1. 00 24. 11 A	
ATOM	4194	CB LEU	543	55. 595 50. 978 54. 660 1. 00 24. 05 A	
ATOM	4195	CG LEU	543	56. 080 51. 474 53. 289 1. 00 22. 45 A	
ATOM	4196	CD1 LEU	543	57. 209 52. 487 53. 475 1. 00 24. 00 A 56. 537 50. 303 52. 441 1. 00 20. 16 A	
ATOM	4197	CD2 LEU	543		
ATOM	4198	C LEU	543	54. 378 53. 131 54. 966 1. 00 24. 37 A 53. 283 52. 819 54. 511 1. 00 25. 72 A	
ATOM	4199	0 LEU	543 544	54. 857 54. 362 54. 896 1. 00 24. 80 A	
ATOM	4200	N LEU CA LEU	544	54. 098 55. 436 54. 278 1. 00 23. 74 A	
ATOM	4201 4202	CB LEU	544	54. 424 56. 757 54. 979 1. 00 23. 92 A	
ATOM ATOM	4202		544	53. 640 58. 003 54. 581 1. 00 22. 62 A	
ATOM	4204		544	52.157 57.743 54.729 1.00 24.91 A	
ATOM	4205		544	54,069 59,166 55,460 1.00 24,25 A	
ATOM	4206		544	54. 403 55. 543 52. 785 1. 00 23. 24 A	
ATOM	4207		544	55.451 56.053 52.400 1.00 23.44 A	
ATOM	4208		· 545	53. 477 55. 049 51. 962 1. 00 21. 43 A	
ATOM	4209	CA ASP	545	53. 595 55. 075 50. 508 1. 00 20. 10 A	
ATOM	4210	CB ASP	545	52.570 54.132 49.902 1.00 20.20 A	
ATOM	4211		545	52. 826 53. 848 48. 444 1. 00 20. 73 A	
ATOM	4212		545	53.175 54.790 47.699 1.00 22.69 A 52.660 52.675 48.044 1.00 19.91 A	
MOTA	4213	OD2 ASP	545	52.660 52.675 48.044 1.00 19.91 A	ı U

	(Continued)					
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4214 4215 4216 4217 4218 4219 4220 4221 4222 4223 4224 4225 4223 4231 4232 4233 4234 4235 4236 4237 4242 4242 4243 4242 4243 4242 4243 4242 4243 4242 4243 4242 4243 4242 4243 4242 4243 4244 4245 4246 4247 4248 4257 4258 4258 4259 4259 4259 4259 4259 4259 4259 4259	O N CAECO CO N CAECO N	VAL VAL VAL TYR TYR TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	545 546 546 546 546 547 547 547 547 547 547 547 547 547 547	FIG. 4 - 87 53. 281 56. 499 50. 078 1. 00 20. 41 52. 149 56. 949 50. 219 1. 00 21. 14 54. 263 57. 201 49. 524 1. 00 19. 56 54. 043 58. 591 49. 157 1. 00 20. 20 54. 867 59. 511 50. 090 1. 00 20. 60 54. 626 60. 966 49. 753 1. 00 20. 01 54. 499 59. 239 51. 533 1. 00 21. 16 54. 320 59. 032 47. 723 1. 00 20. 22 55. 212 58. 513 47. 048 1. 00 22. 79 53. 524 59. 994 47. 267 1. 00 17. 64 53. 702 60. 604 45. 957 1. 00 15. 73 52. 653 60. 155 44. 952 1. 00 13. 49 52. 969 60. 718 43. 589 1. 00 13. 89 52. 160 61. 688 43. 006 1. 00 14. 20 52. 513 62. 274 41. 801 1. 00 13. 67 54. 136 60. 347 42. 921 1. 00 9. 92 54. 492 60. 926 41. 726 1. 00 10. 35 53. 680 61. 890 41. 167 1. 00 12. 20 54. 036 62. 474 39. 973 1. 00 14. 66 53. 522 62. 076 46. 266 1. 00 14. 99 54. 490 62. 834 46. 325 1. 00 14. 47 52. 265 62. 456 46. 479 1. 00 14. 77 51. 879 63. 806 46. 878 1. 00 12. 10 52. 493 64. 109 48. 247 1. 00 9. 78 52. 163 64. 950 45. 923 1. 00 11. 87 52. 250 66. 094 46. 346 1. 00 12. 24 52. 308 64. 660 44. 639 1. 00 13. 59 52. 163 66. 578 43. 696 1. 00 13. 20 54. 306 66. 578 43. 696 1. 00 13. 20 54. 307 66. 884 42. 280 1. 00 15. 91 52. 533 68. 380 42. 280 1. 00 15. 91 52. 533 68. 380 42. 280 1. 00 15. 59 52. 146 68. 592 42. 776 1. 00 15. 03 54. 366 67. 745 42. 915 1. 00 15. 91 52. 533 68. 380 42. 280 1. 00 16. 15 53. 60. 693 69. 794 41. 989 1. 00 15. 59 54. 499 67. 946 42. 532 1. 00 15. 67 54. 366 67. 745 42. 915 1. 00 15. 03 54. 366 67. 745 42. 915 1. 00 15. 03 54. 366 67. 745 42. 915 1. 00 15. 03 54. 366 67. 745 42. 915 1. 00 15. 03 54. 366 67. 745 42. 915 1. 00 15. 03 54. 366 67. 745 42. 915 1. 00 15. 03 54. 366 67. 745 42. 915 1. 00 15. 03 54. 366 67. 745 42. 915 1. 00 15. 03 54. 366 67. 745 42. 915 1. 00 15. 03 54. 366 67. 745 42. 915 1. 00 15. 03 54. 366 67. 745 42. 915 1. 00 15. 03 55. 136 66. 578 43. 573 1. 00 15. 67 56. 693 69. 794 41. 989 1. 00 15. 50 56. 693 69. 794 41. 989 1. 00 15. 50 56. 693 69. 794 41. 989 1. 00 15. 50 57. 66. 6182 64. 796 64. 525 1. 00 16. 53 58. 40. 6184 67. 287 41. 944 1. 00 16. 54 59. 366 67. 314 39. 844	CONCCCCOCCCCCCCCCCONCCCONCCCONCCCONCCCSCO
ATOM	4257	N	SER	552	47. 574 65. 219 42. 856 1. 00 16. 56 A 47. 742 63. 785 42. 933 1. 00 16. 35 A 49. 063 63. 450 43. 613 1. 00 19. 76 A 49. 023 63. 805 44. 987 1. 00 20. 36 A	N
ATOM	4258	CA	SER	552		C
ATOM	4259	CB	SER	552		C
ATOM	4260	OG	SER	552		O
ATOM	4261	C	SER	552	46. 602 63. 202 43. 760 1. 00 17. 72 A 45. 723 63. 929 44. 243 1. 00 17. 55 A SUBSTITUTE SHEET (RULE 26)	C
ATOM	4262	0	SER	552		0

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ATOM	4263		GLN	553	46.632	61.885	43. 926	1.00 17.07	A	N C
ATOM	4264	-	GLN	553	45.628	61.179	44.699	1.00 16.87 1.00 16.43	A A	č
ATOM	4265		GLN	553	44.301	61.090	43. 937 44. 695	1.00 10.43	A	Č
ATOM	4266		GLN	553	43. 249	60. 292		1.00 19.33	A	Č
ATOM	4267		GLN	553	41.844 41.520	60. 468 60. 019	43.066	1.00 20.67	A	Ö
ATOM	4268	OE1		553	41. 520	61.126	44.944	1.00 20.07	A	N
ATOM	4269	NE2		553 553	46.123	59. 781	44. 996	1.00 18.09	A	Č
ATOM	4270		GLN	553	46. 088	58. 915	44. 129	1.00 18.05	A	ŏ
ATOM	4271		GLN LYS	554	46.589	59. 562	46. 221	1.00 10.20	A	N
ATOM ATOM	4272		LYS	554 554	47.075	58. 248	46. 620	1.00 20.69	Ä	Ċ
ATOM	4273 4274		LYS	554	48. 319	58. 387	47. 490	1.00 22.65	Ä	č
ATOM	4275		LYS	554	49. 538	58. 887	46. 733	1.00 24.15	Ä	č
ATOM			LYS	554	50.064	57. 840	45. 765	1.00 25.21	Ä	č
ATOM	4277		LYS	554	50.777	56. 711	46. 503	1.00 24.75	Ä	Č
ATOM	4278		LYS	554	51.472	55. 796	45. 560	1.00 23.89	Ā	N
ATOM	4279		LYS	554	45. 996	57. 472	47. 374	1.00 21.48	A	С
ATOM	4280		LYS	554	46. 108	56. 258	47.549	1.00 22.39	A	0
ATOM	4281	Ň	ALA	555	44.952	58.176	47.807	1.00 20.77	A	N
ATOM	4282	CA	ALA	555	43.849	57.555	48.538	1.00 20.46	A	C
ATOM	4283	CB	ALA	555	43.525	58.376	49.768	1.00 18.05	Α	C
ATOM	4284	C	ALA	555	42.611	57.436	47.643	1.00 21.32	A	C
ATOM	4285	0	ALA	555	41.996	58.442	47. 285	1.00 21.75	Α	0
ATOM	4286	N	ASP	556	42.249	56. 208	47. 283	1.00 21.00	Α	N
ATOM	4287	CA	ASP	556	41.096	55. 981	46. 419	1.00 20.04	A	Ç
ATOM	4288	CB	ASP	556	41.500	56. 151	44.960	1.00 20.02	A	Č
ATOM	4289	CG	ASP	556	42.649	55.255	44. 574	1.00 19.76	A	C
ATOM	4290	0D1		556	42.723	54. 132	45. 115	1.00 19.65	A	0
ATOM	4291	0D2		556	43.470	55.666	43. 723	1.00 21.90	A	0
ATOM	4292	С	ASP	556	40.478	54.603	46.614	1.00 20.18	Ą	C
ATOM	4293	0	ASP	556	40.856	53. 874	47. 523	1.00 19.93	A	0
ATOM	4294	N	THR	557	39.542	54. 246	45. 736	1.00 20.55	A	N
ATOM	4295	CA	THR	557	38. 835	52.965	45. 820	1.00 22.31	A	C
ATOM	4296	CB	THR	557	37. 331	53. 154	45. 578	1.00 21.37	A	C
ATOM	4297		THR		37.130	53. 580	44. 224	1.00 21.50	A	0 C
ATOM	4298		THR		36. 754	54. 201 51. 898	46. 523 44. 826	1.00 21.28 1.00 23.72	A A	C
ATOM	4299	C	THR	557 557	39. 294			1.00 25.32	A	
ATOM	4300			557 558			44. 194	1.00 23.32	A	N N
ATOM	4301	N CA	VAL VAL	558	40. 441 40. 931	52. 105 51. 143	43. 219	1.00 22.53	A	C
ATOM	4302 4303	CB	VAL	558	40. 931	51. 143	42. 294	1.00 22.67	A	Č
ATOM ATOM	4303		VAL	558	42. 540	, 50. 783	41. 323	1.00 19.20	A	č
ATOM	4305		VAL	558	41. 323	52. 964	41.547	1.00 21.12	A	Č
ATOM	4306	C	VAL	558	41.544	49. 906	43. 871	1.00 23.92	Ä	Č
ATOM	4307	ŏ	VAL	558	42. 246	50.005	44. 871	1.00 23.71	Ä	· ŏ
ATOM	4308	N	PHE	559	41. 261	48. 734	43. 312	1.00 25.05	Ä	Ň
ATOM	4309	CA	PHE	559	41.815	47. 492	43. 841	1.00 25.45	Ä	Ċ
ATOM	4310	CB	PHE	559	40. 855	46. 326	43. 584	1.00 24.60	Ä	č
ATOM	4311	CG	PHE	559	41.476	44. 977	43. 808	1.00 24.75	Ä	Č
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					FIC	G. 4	- 89			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4312 4313 4314 4315 4316 4317 4318 4320 4321 4322 4323 4324 4325	CD2 CE1 CE2 CZ C O N CA CB CG CD NE CZ	PHE PHE PHE PHE ARG ARG ARG ARG ARG	559 559 559 559 559 560 560 560 560 560	42. 192 41. 382 42. 810 41. 995 42. 709 43. 158 43. 250 44. 188 45. 508 46. 398 45. 869 46. 885 46. 269	44. 352 44. 352 43. 118 43. 125 42. 507 47. 210 47. 246 46. 912 46. 644 47. 892 49. 140 50. 285 51. 536 52. 391	- 8 9 42. 799 45. 044 43. 021 45. 276 44. 266 43. 170 41. 943 43. 962 43. 397 43. 510 42. 802 42. 869 43. 310 42. 515	1. 00 25. 70 1. 00 25. 27 1. 00 28. 04 1. 00 24. 71 1. 00 26. 38 1. 00 26. 14 1. 00 27. 21 1. 00 24. 72 1. 00 23. 52 1. 00 20. 68 1. 00 19. 21 1. 00 17. 64 1. 00 20. 38 1. 00 20. 51	A A A A A A A A A A A A A A A A A A A	C C C C C C C C C C C C C
ATOM ATOM	4326 4327	NH1		560 560	45.543	52. 149 53. 468	41.218 43.022	1.00 26.51 1.00 20.25	Α	N N
ATOM ATOM ATOM ATOM ATOM	4328 4329 4330 4331 4332	C O N CA CB	ARG ARG LEU LEU LEU	560 560 561 561 561	46. 274 46. 112 47. 111 47. 968	45. 451 45. 081 44. 856 43. 740 42. 523	43. 980 45. 145 43. 136 43. 511 42. 635	1.00 20.23 1.00 24.37 1.00 24.84 1.00 23.62 1.00 20.95 1.00 18.87	A A A A A	C O N C C
ATOM	4333	CG	LEU	561	46.283	41.916	42.773	1.00 20.60	A	C
ATOM ATOM	4334 4335		LEU LEU	561 561		40. 749 41. 460	41.803 44.203	1.00 19.75 1.00 17.53	A A	C C
ATOM	4336	C	LEU	561	49. 380	44. 255	43.246	1.00 20.00	A	C
ATOM ATOM	4337 4338	O N	LEU ASN	561 562		44. 152 44. 822	42. 133 44. 274	1.00 20.19 1.00 18.97	A A	O N
ATOM	4339	CA	ASN	562	51.335	45. 392	44.142	1.00 18.20.	Α	C
ATOM ATOM	4340 4341	CB CG	ASN ASN	562 562		46. 907 47. 491	44. 028 45. 148	1.00 16.72 1.00 17.45	A A	C C
ATOM	4342		ASN	562	49. 881	48.610	45.054	1.00 19.63	A	0
ATOM ATOM	4343 4344	NDZ C	ASN ASN	562 562		46. 729 45. 035	46. 223 45. 289	1.00 18.39 1.00 18.48	A A	N C
ATOM	4345	0	ASN	562	52.055	44.098	46.056	1.00 19.79	A	0
ATOM ATOM	4346 4347	N CA	TRP TRP	563 563		45. 793 45. 548	45. 400 46. 434	1.00 17.98 1.00 17.62	A A	N C
ATOM	4348	CB	TRP	563	55. 538	46.537	46. 290	1.00 16.04	A	Č
ATOM ATOM	4349 4350	CD2	TRP TRP	563 563		46. 249 47. 200	47. 178 47. 968	1.00 15.76 1.00 13.80	A	C
ATOM	4351	CE2	TRP	563		46. 500	48. 602	1.00 13.60	A A	C C
ATOM ATOM	4352 4353	CE3 CD1		563		48. 575	48. 198	1.00 13.46	A	С
ATOM	4354	NE1		563 563		45. 041 45. 189	47. 361 48. 217	1.00 12.65 1.00 11.34	A A	C N
ATOM	4355	CZ2	TRP	563	59.439	47.128	49.453	1.00 14.40	Α	С
ATOM ATOM	4356 4357	CZ3 CH2		563 563		49. 204 48. 476	49. 046 49. 664	1.00 16.29 1.00 14.18	A A	C C
ATOM	4358	С	TRP	563	53.728	45. 672	47.809	1.00 17.48	A	C
ATOM ATOM	4359 4360	0 N	TRP ALA	563 564		44. 910 46. 620	48. 720 47. 953	1. 00 18. 93 1. 00 16. 80	Α	0
117 014	1000	**	ישעה	004	04.010	10.040	¥1.300	1.00 10.00	Α	N

F I G. 4 - 90											
ATOM	4361	CA	ALA	564	ļ	F 1 52.151	46. 838	49. 232	1.00 17.11	A	С
ATOM	4362		ALA	564		51.248	48.068	49. 153	1.00 16.72	A	Ċ
ATOM	4363		ALA	564		51.341	45.616	49.655	1.00 17.89	Α	С
ATOM	4364		ALA	564		51.322	45. 256	50.834	1.00 15.94	Α	0
ATOM	4365	Ň	THR	565		50.676	44. 983	48.691	1.00 18.77	Α	N
ATOM	4366	CA	THR	565		49.870	43.801	48.977	1.00 19.59	Α	C
ATOM	4367	CB	THR	565		49.368	43. 131	47.689	1.00 20.01	A	C
ATOM	4368			565		48.606	44.069	46.922	1.00 19.76	A	0 .
ATOM	4369	CG2		565		48.496	41.922	48. 027	1.00 19.34	A	C
ATOM	4370	C	THR	565		50.718	42. 793	49. 739	1.00 21.27	A	C
ATOM	4371	0	THR	565		50. 290	42. 252	50.760	1.00 22.29	A	0
ATOM	4372	N	TYR	566		51.924	42. 548	49. 234	1.00 22.25	A	N C
ATOM	4373	CA	TYR	566		52. 848	41.615	49.864	1.00 23.40	A	C
ATOM	4374	CB	TYR	566		54.029	41.324	48. 923	1.00 25.18 1.00 25.40	A	C C
ATOM	4375	CG	TYR	566		55.369	41.218 42.262	49. 616 49. 547	1.00 25.40	A A	Č
ATOM	4376			566		56. 297 57. 513	42. 202	50. 226	1.00 26.85	A	č
ATOM	4377	CE1		566 566		55.690	42. 190	50. 382	1.00 26.89	A	Č
ATOM	4378	CD2 CE2		566		56. 903	40. 101	51.073	1.00 20.33	A	č
ATOM	4379 4380	CZ	TYR	566		57. 809	41.074	50.991	1.00 30.16	A	č
ATOM ATOM	4381	OH	TYR	566		58. 997	40.998	51.688	1.00 32.61	A	ŏ
ATOM	4382	C	TYR	566		53. 369	42.116	51. 212	1.00 23.06	A	č
ATOM	4383	Ö	TYR	566		53. 458	41.350	52.170	1.00 21.96	A	Ö
ATOM	4384	N	LEU	567		53. 716	43. 396	51. 288	1.00 23.28	A	Ň
ATOM	4385		LEU	567		54. 237	43.949	52.532	1.00 24.50	Α	C
ATOM	4386	CB	LEU	567		54. 588	45.429	52.359	1.00 22.74	Α	С
ATOM	4387	ĊĠ	LEU	567		55.717	45.769	51.378	1.00 23.15	Α	С
ATOM	4388		LEU	567		55. 833	47.279	51.263	1.00 20.37	Α	C
ATOM	4389		LEU	567		57.038	45.158	51.850	1.00 21.42	Α	С
ATOM	4390	C	LEU	567		53. 243	43.786	53.675	1.00 26.32	Α	С
ATOM	4391	0	LEU	567		53.635	43.595	54. 824	1.00 27.44	Α	0
ATOM	4392	N	ALA	568		51.955	43.857	53. 361	1.00 26.96	A	N
ATOM	4393	CA	ALA	568		50.930	43.712	54. 383	1.00 27.44	A	C
ATOM	4394	CB	ALA	568		49.684	44. 481	53. 984	1.00 26.54	A	C
ATOM	4395	C	ALA	568		50.584	42. 242	54.606	1.00 29.12	Ą	C
ATOM	4396		ALA	568		50.483		55. 748	1.00 28.80	A	0
ATOM	4397	N	SER	569		50.417	41.506	53. 509	1.00 28.58	A	N
ATOM	4398	CA	SER	569		50.062	40.094	53. 586	1.00 28.31	A	C
ATOM	4399	CB	SER	569		49.750	39.553	52. 191	1.00 28.85	A	C
ATOM	4400	0G	SER	569		49. 420	38. 174	52. 247 54. 236	1.00 30.69 1.00 27.43	A A	0 C
ATOM	4401	C	SER	569		51.110	39. 204 38. 427	55. 133	1.00 27.43	A	0
MOTA	4402 4403	0	SER	569 570		50.800 52.350	39. 311	53. 781	1.00 27.24	Ä	N
ATOM	4403 4404	N CA	THR THR	570 570		53. 420	38. 483	54. 314	1.00 27.02	Ä	C
ATOM ATOM	4404	CB	THR	570		54. 410	38. 094	53. 199	1.00 26.90	A	Č
ATOM	4406	0G1		570		53. 749	37. 250	52. 248	1.00 27.63	Ä	ŏ
ATOM	4407		THR	570		55. 611	37. 369	53. 774	1.00 23.88	A	Č
ATOM	4408	C	THR	570		54. 203	39. 110	55. 459	1.00 27.34	A	č
ATOM	4409	Ö	THR	570		54. 362	38. 496	56. 512	1.00 30.01	Ā	Ö
TIT OU	1100	v		3.0							

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FIG. 4-91											
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4411 CA 4412 CB 4413 CG 4414 CD 4415 OE1 4416 OE2 4417 C 4418 O 4419 N 4420 CA 4421 CB 4422 CG 4423 OD1 4424 ND2 4425 C 4426 O 4427 N 4428 CA 4429 CB 4430 CG2 4431 CG1 4432 CD1 4433 C 4434 O 4435 N 4436 CA 4437 CB 4438 CG2 4431 CG1 4432 CD1 14431 CG1 14432 CD1 14443 CG1 14444 CA 14442 O 14443 N 14444 CA 14443 N 14444 CA	GLU 571 GLU 571 GLU 571 GLU 571 GLU 571 ASN 572 ALE 573 ILE 574 ILE 575 ILE 575	54. 686 40. 32 55. 480 41. 02 56. 402 42. 04 57. 287 41. 47 58. 238 40. 32 58. 582 40. 42 58. 656 39. 52 54. 643 41. 71 55. 188 42. 363 53. 324 41. 576 52. 425 42. 193 52. 557 41. 486 52. 139 40. 033 52. 711 39. 183 52. 683 43. 681 52. 642 44. 178 53. 208 45. 824 54. 396 46. 198 54. 715 47. 669 55. 622 45. 365 56. 805 45. 636 51. 992 46. 621 51. 353 46. 249 51. 681 47. 718 50. 557 48. 555 49. 926 49. 297 48. 794 48. 968 51. 064 49. 619 51. 799 50. 524 50. 683 49. 521 51. 128 50. 517	55. 253 1 56. 259 1 55. 583 1 54. 473 1 54. 966 1 56. 164 1 54. 158 1 57. 329 1 58. 213 1 57. 247 1 58. 223 1 59. 569 1 59. 569 1 59. 569 1 57. 321 1 57. 32	. 00 26. 71 . 00 25. 23 . 00 24. 64 . 00 25. 43 . 00 27. 45 . 00 28. 11 . 00 24. 50 . 00 24. 29 . 00 24. 39 . 00 24. 96 . 00 25. 44 . 00 29. 03 . 00 25. 32 . 00 25. 55 . 00 25. 55 . 00 25. 55 . 00 25. 48 . 00 24. 87 . 00 24. 87 . 00 25. 36 . 00 26. 14 . 00 25. 88 . 00 26. 06 . 00 27. 12 . 00 28. 97 . 00 25. 92 . 00 24. 87	A A A A A A A A A A A A A A A A A A A	(Continued) N C C C C C C C C C C C C C C C C C C				
ATOM ATOM		AL 575 AL 575	51. 128 50. 517 51. 387 49. 904 51. 973 50. 966 52. 320 48. 707	52.569 1. 51.644 1.	00 24.87 00 24.76 00 20.17 00 22.12	A A A A	C C C				
ATOM ATOM ATOM ATOM ATOM ATOM	4448 C V 4449 O V 4450 N A 4451 CA A 4452 CB A 4453 C A	AL 575 AL 575 LA 576 LA 576 LA 576 LA 576 LA 576	50. 054 51. 585 48. 929 51. 312 50. 403 52. 804 49. 456 53. 893 49. 255 54. 477 49. 879 54. 988 51. 056 55. 139	53. 837 1. 6 53. 405 1. 6 54. 216 1. 6 54. 152 1. 6 55. 540 1. 6 53. 180 1. 6	00 25. 21 00 25. 63 00 23. 75 00 23. 56 00 23. 43 00 24. 06	A A A A A A	C O N C C C				
ATOM ATOM	4456 CA SI 4457 CB SI	ER 577 ER 577 ER 577 ER 577	48. 888 55. 740 49. 095 56. 852 48. 793 56. 428 49. 750 55. 475	52.710 1.0 51.796 1.0 50.362 1.0	00 24.49 00 23.11 00 23.06	A A A A	N C C O				

					- FI	G. 4	- 92			(Continued	ł)
ATOM	4459	С	SER	577	48. 149	57.947	52. 248	1.00 22.90	Α	С	
ATOM	4460	0	SER	577	47.075	57.662	52.768	1.00 24.22	Α	0	
ATOM	4461	N	PHE	578	48.546	59.196	52.046	1.00 23.49	Α	N	
ATOM	4462	CA	PHE	578	47. 748	60. 337	52.479	1.00 21.77	Α	C	
ATOM	4463	CB	PHE	578	48. 313	60.829	53.804	1.00 21.41	A	C	
ATOM	4464		PHE	578	47. 585	62.005	54. 383	1.00 22.79	A	C	
MOTA	4465		PHE	578	46. 429	61.820	55. 144	1.00 20.60	Ą	C	
ATOM	4466		PHE	578	48. 080	63. 291	54. 209	1.00 19.79	A	C	
ATOM	4467		PHE	5 7 8	45. 783	62.901	55. 730	1.00 21.26	A	C	
ATOM	4468		PHE	578	47.441	64. 381	54.790	1.00 20.94	A	C	
ATOM	4469	CZ	PHE	578 578	46. 288	64. 186	55. 556	1.00 20.70	A	C C	
ATOM	4470	C	PHE	578	47.723	61.502 61.909	51.480 50.973	1.00 21.14 1.00 21.08	A A	0	
ATOM	4471	O N	PHE ASP	578 579	48. 766 46. 533	62.041	51. 212	1.00 21.08	A	N	
ATOM ATOM	4472 4473	IN CA	ASP	579	46. 389	63.173	50. 302	1.00 13.03	A	Č	
ATOM	4474	CB	ASP	579	45. 191	62. 985	49. 371	1.00 17.01	A	Č	
ATOM	4475	CG	ASP	579	45. 334	61.777	48. 455	1.00 21.86	A	č	
ATOM	4476		ASP	579	46. 424	61.583	47.873	1.00 22.87	Ä	Ö	
ATOM	4477		ASP	579	44. 342	61.024	48. 299	1.00 23.17	Ā	Ö	
ATOM	4478	C	ASP	579	46. 211	64.474	51.092	1.00 18.10	Α	C	
ATOM	4479	Ō	ASP	579	45. 103	64.823	51.493	1.00 20.42	Α	0	
ATOM	4480	N	GLY	580	47. 306	65. 189	51.313	1.00 17.22	Α	N	
ATOM	4481	CA	GLY	580	47. 238	66.439	52.044	1.00 15.14	A	С	
ATOM	4482	C	GLY	580	47. 065	67.610	51.098	1.00 16.53	Α	С	
ATOM	4483	0	GLY	580	46. 544	67.462	49. 993	1.00 17.18	A	0 .	
ATOM	4484	N	ARG	581	47. 495	68. 786	51.528	1.00 15.90	A	N	
ATOM	4485	CA	ARG	581	47. 377	69.970	50. 701	1.00 15.52	A	C	
ATOM	4486	CB	ARG	581	47. 956	71.172	51.444	1.00 16.17	A	C	
ATOM	4487	CG	ARG	581	47.072	71.645	52. 585	1.00 16.05	A	C	
ATOM	4488	CD	ARG	581	47. 756	72. 653 71. 990	53. 467 54. 441	1.00 14.87 1.00 18.25	A A	C N	
ATOM	4489 4490	NE CZ	ARG ARG	581 581	48. 617 49. 321	72.624	55. 375	1.00 18.23	A	C	
ATOM ATOM	4490		ARG	581	49. 268	73. 952	55. 463	1.00 20.41	A	N	
ATOM	4492		ARG	581	50.075	71. 933	56. 224	1.00 25.41	A	N	
ATOM	4493	C	ARG	581	48. 107	69. 742	49. 386	1.00 17.75	A	Ĉ	
ATOM	4494	ŏ	ARG	581	49. 193	69. 158	49. 357	1.00 17.49	Ä	Ŏ	
ATOM	4495	Ň	GLY	582	47. 495	70. 192	48. 295	1.00 18.96	Ä	Ň	
ATOM	4496	CA	GLY	582	48.094	70.022	46.987	1.00 17.63	Α	. C	
ATOM	4497	C	GLY	582	47.511	68.842	46. 231	1.00 18.54	Α	C	
ATOM	4498	0	GLY	582	47.673	68.757	45.017	1.00 18.99	Α	0	
ATOM	4499	N	SER	583	46.842	67. 923	46. 925	1.00 18.00	Α	N	
MOTA	4500	CA	SER	583	46. 258	66.765	46. 247	1.00 18.46	Α	C	
ATOM	4501	CB	SER	583	45. 842	65.700	47. 269	1.00 18.34	A	C	
ATOM	4502	0G	SER	583	45.058	66. 253	48. 303	1.00 19.12	A	0	
ATOM	4503	C	SER	583	45.068	67. 218	45. 392	1.00 18.03	A	C	
ATOM	4504	0	SER	583	44.601	68. 344	45. 536	1.00 17.42	A	0	
ATOM	4505	N	GLY	584	44. 570	66. 355	44. 510	1.00 17.84	A	N	
ATOM	4506	CA	GLY	584 584	43. 481	66. 779	43.637	1.00 19.22 1.00 19.49	A A	C C	
ATOM	4507	С	GLY	584	42.052	66. 293	43. 827	1.00 13.43	A	U	

FIG. 4 - 93												
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4509 4510 4511 4511 4511 4511 4511 4511 4511	N CAB CCD CE CCZ OH C O N CAB CCD OE CCZ OH C O N CAB CCD OE CCZ OH C O N CAB CCD OD C O N CAB CCD OD CON CAB CCD ON CAB	TYR TYR TYR TYR TYR TYR TYR TYR GLN GLN GLN GLY GLY ASP ASP LYS	584 585 585 585 585 585 585 586 586 586 586	41. 724 65. 570 44. 767 1. 00 21. 57 41. 191 66. 735 42. 917 1. 00 19. 76 39. 782 66. 362 42. 906 1. 00 18. 53 39. 673 64. 859 42. 663 1. 00 18. 57 40. 578 64. 401 41. 550 1. 00 18. 83 40. 439 64. 914 40. 260 1. 00 19. 48 41. 300 64. 533 39. 235 1. 00 18. 11 41. 606 63. 490 41. 789 1. 00 19. 81 42. 476 63. 100 40. 769 1. 00 17. 71 42. 313 63. 626 39. 497 1. 00 18. 76 43. 150 63. 232 38. 481 1. 00 20. 70 38. 997 66. 751 44. 152 1. 00 18. 81 38. 046 66. 067 44. 521 1. 00 17. 85 39. 382 67. 861 44. 783 1. 00 20. 25 38. 708 68. 345 45. 986 1. 00 20. 04 40. 781 66. 095 48. 363 1. 00 24. 77 40. 441 66. 029 49. 548 1. 00 23. 60 42. 044 65. 919 47. 962 1. 00 23. 60 42. 044 65. 919 47. 962 1. 00 23. 83 38. 707 71. 969 44. 853 1. 00 21. 24 40. 073 72. 623 44. 883 1. 00 21. 25 41. 415 74. 580 44. 397 1. 00 21. 25 41. 415 74. 580 44. 397 1. 00 21. 25 41. 415 74. 580 44. 397 1. 00 22. 09 41. 287 75. 763 43. 382 1. 00 22. 09 41. 287 75. 763 43. 382 1. 00 22. 29 41. 130 75. 086 46. 716 1. 00 23. 11 41. 190 75. 562 47. 998 1. 00 22. 09 41. 287 75. 763 43. 382 1. 00 22. 97 40. 441 65. 76. 213 41. 211 1. 00 25. 77 41. 157 74. 155 41. 599 1. 00 23. 83 43. 121 75. 471 45. 762 1. 00 23. 83 43. 121 75. 471 45. 762 1. 00 23. 77 41. 620 75. 562 47. 998 1. 00 22. 97 40. 599 75. 616 49. 037 1. 00 24. 26 40. 994 76. 173 50. 365 1. 00 22. 97 40. 599 76. 614 15. 14. 599 1. 00 23. 77 41. 620 75. 562 47. 998 1. 00 22. 97 40. 599 76. 616 49. 037 1. 00 22. 97 41. 157 76. 638 52. 784 1. 00 35. 08 40. 457 76. 638 52. 784 1. 00 35. 08 40. 457 76. 638 52. 784 1. 00 35. 08 40. 447 75. 340 48. 468 1. 00 22. 93 41. 287 75. 766 38. 81. 1. 00 22. 93 42. 444 73. 326 48. 217 1. 00 21. 76 42. 737 70. 956 48. 846 1. 00 23. 17 42. 494 73. 326 48. 217 1. 00 21. 76 42. 737 70. 956 48. 846 1. 00 22. 93 43. 711 75. 032 48. 607 1. 00 21. 94 44. 901 71. 025 50. 126 1. 00 21. 94 41. 901 71. 025 50. 126 1. 00 22. 93 43. 710 71. 956 48. 846 1. 00 22. 93 44. 1. 901 71. 025 50. 126 1. 00 21. 94 41. 900 69. 720 50. 478 1. 00 22. 22	N C						

F I G. 4 - 94											
					F I (J. 4	94				
ATOM	4557	C	ILE	590	44. 537	72.093	47.562	1.00 22.32	A	C	
ATOM	4558	0	ILE	590	45.711	71.960	47. 901	1.00 23.51	A	0 N	
ATOM	4559		MET	591	44. 157	72.071	46. 291 45. 232	1.00 21.59 1.00 21.59	A A	N C	
ATOM	4560		MET	591 591	45. 127 44. 406	71.846 71.567	43. 232	1.00 21.80	A	č	
ATOM	4561 4562	CB CG	MET MET	591	45. 309	71.000	42. 838	1.00 21.85	A	č	
ATOM ATOM	4563	SD	MET	591	44. 403	70.746	41.309	1.00 22.76	A	Š	
ATOM	4564	CE	MET	591	44. 237	72. 436	40. 732	1.00 22.84	Α	C	
ATOM	4565	C	MET	591	46.112	72.997	45.051	1.00 21.43	Α	C	
ATOM	4566	Ŏ	MET	591	47. 289	72.771	44. 791	1.00 19.25	A	0	
ATOM	4567	N	HIS	592	45. 636	74. 228	45. 200	1.00 21.21	A	N	
ATOM	4568		HIS	592	46. 502	75.386	45. 035	1.00 21.43	A	C	
ATOM	4569		HIS	592	45. 713	76. 560	44. 455	1.00 22.32	A	C	
ATOM	4570		HIS	592	45. 296	76. 361	43.032	1.00 24.65 1.00 26.25	A A	C C	
ATOM	4571		HIS	592	45.604	75. 390 77. 243	42. 139 42. 368	1.00 25.75	A	N N	
ATOM	4572	ND1		592	44. 471 44. 289	76. 825	41.128	1.00 25.75	A	Ç	
ATOM	4573		HIS HIS	592 592	44. 265 44. 965	75. 703	40. 962	1.00 25.78	Ä	Ň ·	
ATOM ATOM	4574 4575	C	HIS	592 592	47. 197	75. 817	46. 319	1.00 21.38	Ä	Ĉ	
ATOM	4576	0	HIS	592	47. 842	76. 865	46. 362	1.00 20.84	Ä	Ō	
ATOM	4577	N	ALA	593	47.076	75.012	47.367	1.00 21.76	A	N	
ATOM	4578	CA	ALA	593	47.732	75.349	48.628	1.00 20.43	Α	C	
ATOM	4579	CB	ALA	593	47.360	74.349	49.710	1.00 18.24	A	C	
ATOM	4580	C	ALA	593	49. 241	75. 361	48. 427	1.00 19.92	A	C	
ATOM	4581	0	ALA	593	49.940	76. 126	49.081	1.00 21.91	A	0	
ATOM	4582	N	ILE	594	49. 736	74. 522	47.518	1.00 19.47	A	N	
ATOM	4583	CA	ILE	594	51.176	74. 446	47. 248	1.00 20.49	A	C	
ATOM	4584	CB	ILE	594	51.617	73. 021	46.816	1.00 19.36	A A	C C	
ATOM	4585		ILE	594	51.467	72. 051 72. 581	47. 966 45. 590	1.00 19.38 1.00 21.33	A	C	
ATOM	4586		ILE ILE	594 594	50. 814 50. 951	71. 106	45. 243	1.00 22.55	A	č	
ATOM ATOM	4587 4588	CDI	ILE	594 594	51.658	75. 410	46.169	1.00 19.88	A	č	
ATOM	4589	Ö	ILE	594	52. 849	75. 434	45.854	1.00 17.79	A	Ö	
ATOM	4590	N	ASN	595	50. 746	76. 200	45.606	1.00 20.03	Α	N	
ATOM	4591	CA	ASN	595	51.119	77.137	44.547	1.00 21.76	Α	С	
ATOM	4592		ASN	595	49. 977	78. 114	44.265	1.00 20.68	Α	C	
ATOM	4593	CG	ASN	595	50. 300	79.072	43. 128	1.00 21.80	A	C	
ATOM	4594	0D1	ASN	595	50.640	78.652	42.024	1.00 22.78	A	0	
ATOM	4595		ASN	595	50. 191	80. 364	43. 394	1.00 22.74	A	N	
ATOM	4596	C	ASN	595	52.395	77. 921	44. 860	1.00 22.25	A	C	
ATOM	4597	0	ASN	595	52. 442	78. 688	45. 824	1.00 22.44 1.00 22.52	A	0 N	
ATOM	4598	N CA	ARG	596	53. 421 54. 726	77. 715 78. 378	44. 031 44. 171	1.00 22.32	A A	N C	
ATOM	4599	CA CB	ARG ARG	596 596	54. 720 54. 550	79. 898	44. 141	1.00 22.41	A	Č	
ATOM	4600 4601	CG	ARG	596	53. 894	80. 426	42. 880	1.00 21.20	A	č	
ATOM ATOM	4602	CD	ARG	596	53. 398	81.856	43.096	1.00 22.01	A	č	
ATOM	4603	NE	ARG	596	54. 479	82. 760	43. 482	1.00 20.88	A	N	
ATOM	4604		ARG	596	55. 467	83. 112	42.671	1.00 21.35	Α	С	
ATOM	4605		ARG	596	55. 498	82. 635	41.431	1.00 22.62	A	N	

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					FIG. 4-95	(Continued
ATOM	4606		ARG		56. 427 83. 924 43. 096 1. 00 19. 92 A	N
ATOM	4607	C	ARG		55. 492 77. 982 45. 440 1. 00 21. 53 A	C
ATOM	4608	0	ARG		56. 482 78. 611 45. 804 1. 00 20. 59 A	0
ATOM	4609	N	ARG		55. 046 76. 930 46. 107 1. 00 21. 66 A	N
ATOM	4610	CA	ARG	597	55. 705 76. 512 47. 331 1. 00 21. 98 A	Ċ
ATOM	4611	CB	ARG	597	54. 943 77. 061 48. 539 1. 00 23. 55 A	Č
ATOM	4612	CG	ARG	597	55. 184 78. 547 48. 776 1. 00 28. 20 A	C
ATOM	4613	CD	ARG	597	56. 611 78. 813 49. 264 1. 00 30. 86 A	Ç
ATOM ATOM	4614	NE C7	ARG	597 507	56. 891 80. 239 49. 414 1. 00 34. 81 A	N
ATOM	4615	CZ	ARG	597	57. 074 81. 088 48. 401 1. 00 36. 01 A	C
ATOM	4616 4617		ARG ARG	597 597	57.011 80.670 47.142 1.00 33.57 A	N
ATOM	4618	C	ARG	597	57. 326 82. 365 48. 650 1. 00 37. 36 A 55. 869 75. 011 47. 458 1. 00 20. 79 A	N
ATOM	4619	0	ARG	597	EE EOO	C
ATOM	4620	N	LEU	598	FC 100 F1 000 10 101 1 00 10 11	O N
ATOM	4621	CA	LEU	598	56.400 74.398 46.404 1.00 19.44 A 56.649 72.963 46.387 1.00 18.48 A	C
ATOM	4622	CB	LEU	598	FR 140 FR F/F 4F 000 4 00 10 00	C
ATOM	4623	CG	LEU	598	57.142 72.545 45.003 1.00 18.20 A 56.119 72.007 43.994 1.00 19.27 A	C
ATOM	4624		LEU	598	54. 800 72. 731 44. 107 1. 00 19. 49 A	C
ATOM	4625		LEU	598	56.691 72.135 42.595 1.00 18.24 A	C
ATOM	4626	C	LEU	598	57. 692 72. 617 47. 450 1.00 19. 10 A	č
ATOM	4627	0	LEU	598	58.644 73.363 47.679 1.00 19.27 A	ŏ
ATOM	4628	N	GLY	599	57.506 71.485 48.108 1.00 19.24 A	Ň
ATOM	4629	CA	GLY	599	58. 440 71. 090 49. 138 1. 00 20. 34 A	Ċ
ATOM	4630	C	GLY	599	58.055 71.622 50.508 1.00 21.76 A	č
ATOM	4631	0	GLY	599	58. 882 71. 640 51. 422 1. 00 23. 58 A	Ö
ATOM	4632	N	THR	600	56.811 72.061 50.666 1.00 21.02 A	N
ATOM	4633	CA	THR	600	56.381 72.578 51.958 1.00 21.20 A	C
ATOM	4634	CB	THR	600	56.039 74.082 51.874 1.00 21.28 A	C
ATOM	4635		THR	600	54.887 74.271 51.052 1.00 25.68 A	0
ATOM	4636		THR	600	57. 192 74. 856 51. 264 1. 00 21. 23 A	C
ATOM	4637	C	THR	600	55. 201 71. 810 52. 557 1. 00 21. 38 A	C
ATOM	4638	0	THR	600	55. 386 70. 724 53. 100 1. 00 22. 42 A	0
ATOM	4639	N	PHE	601	53. 993 72. 356 52. 446 1. 00 21. 18 A	N
ATOM ATOM	4640	CA	PHE	601	52. 809 71. 721 53. 022 1. 00 22. 09 A	C
ATOM	4641	CB	PHE	601	51.540 72.498 52.649 1.00 24.93 A	C
ATOM	4642 4643	CG	PHE	601	51.556 73.935 53.077 1.00 26.21 A	Č
ATOM	4644		PHE PHE	601	51.052 74.923 52.236 1.00 28.07 A	C
ATOM	4645	CE1		601 601	52.105 74.308 54.299 1.00 26.83 A	C
ATOM	4646	CE2		601	51.100 76.271 52.603 1.00 29.10 A	C
ATOM	4647	CZ	PHE	601	52.160 75.650 54.680 1.00 28.02 A 51.658 76.636 53.830 1.00 28.61 A	C
ATOM	4648	C	PHE	601		C
ATOM	4649	Ö	PHE	601	EO 00=	C
ATOM	4650	N	GLU	602	FO 001 001 0-	0 N
ATOM	4651		GLU	602	FO 510	N
ATOM	4652		GLU	602	FO 000	C
ATOM	4653		GLU	602	E4 000 40 FFD 40 0F1 4 00 0F 44	C C
ATOM	4654		GLU	602	54. 396 68. 559 48. 974 1. 00 27. 44 A 54. 872 70. 002 48. 893 1. 00 29. 71 A	C
					72.512 10.002 10.000 1.00 20.11 M	U

FIG. 4-96										
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4655 4656 4657 4658 4669 4661 4662 4663 4664 4665 4666 4667 4670 4671 4672 4673 4674 4675 4676 4677 4678	CCON CA CB CGCO N CA CB CG CD OE1 CGC CON CA CB CG CD OE2 CCON CA CB CG CD OD2	GLU GLU VAL VAL VAL VAL VAL GLU GLU GLU GLU GLU GLU ASP ASP ASP ASP	602 602 602 603 603 603 603 604 604 604 604 604 604 605 605 605 605 605	54. 751 55. 379 53. 663 53. 386 54. 777 55. 772 57. 159 58. 165 57. 603 55. 373 55. 009 54. 594 54. 322 55. 572 56. 449 57. 505 56. 083 53. 349 53. 349 53. 349 53. 349 54. 594 57. 505 56. 083 57. 603 58. 151 59. 003 50. 003 50. 003 50. 003 50. 003	70. 743 70. 392 67. 657 66. 473 68. 229 67. 468 68. 133 67. 365 68. 193 67. 350 66. 265 68. 481 68. 518 69. 964 70. 808 70. 355 70. 989 67. 786 67. 021 67. 436 68. 832 69. 267 69. 499	49. 891 47. 822 51. 698 51. 899 52. 146 52. 897 52. 800 53. 649 51. 335 54. 364 54. 946 54. 951 56. 341 56. 770 56. 924 58. 091 58. 328 58. 773 56. 553 57. 517 55. 650 55. 785 54. 713 54. 963 54. 215 55. 914	1. 00 31. 66 1. 00 31. 46 1. 00 21. 67 1. 00 22. 33 1. 00 20. 78 1. 00 20. 76 1. 00 18. 99 1. 00 15. 00 1. 00 15. 21 1. 00 21. 85 1. 00 20. 44 1. 00 24. 70 1. 00 27. 84 1. 00 30. 83 1. 00 37. 92 1. 00 43. 63 1. 00 46. 30 1. 00 45. 85 1. 00 27. 28 1. 00 28. 68 1. 00 25. 72 1. 00 24. 61 1. 00 23. 36 1. 00 23. 15 1. 00 21. 27	A A A A A A A A A A A A A A A A A A A	(Continued) 0 0 C 0 N C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4681 4682 4683 4684 4685 4686 4687 4688 4690 4691 4692 4693 4694 4695 4697 4698 4699 4700 4701 4702 4703	C O N CA CB CG2 CG1 CD1 C O N CA CB CG2 CG2 CG1 CCD1 C C O N CA CB CC CG2 CG CCD1 C C O N CA CCB CC CCB CCC CCC CCC CCC CCC CCC C	GLN GLN ILE ILE ILE ILE ILE	605 606 606 606 606 606 606 606 607 607 607	51. 379 50. 646 52. 394 52. 704 53. 788 53. 305 52. 206 52. 373 51. 075 53. 207 52. 838 54. 059 54. 607 55. 639 56. 165 56. 789 57. 796 53. 359 52. 619 51. 508 50. 705 49. 578	65. 515 64. 779 65. 051 63. 627 63. 302 63. 332 62. 321 61. 122 62. 801 63. 268 62. 238 64. 129 63. 915 65. 002 64. 778 64. 977 66. 086 63. 963 63. 093 64. 978 65. 099 66. 379 66. 581	55. 783 56. 439 55. 063 55. 056 54. 026 52. 596 52. 330 52. 560 51. 840 56. 447 57. 002 57. 001 58. 337 58. 702 60. 116 57. 694 57. 881 59. 355 60. 226 59. 239 60. 164 59. 936	1. 00 26. 18 1. 00 28. 35 1. 00 26. 16 1. 00 25. 29 1. 00 24. 18 1. 00 24. 92 1. 00 24. 81 1. 00 25. 31 1. 00 25. 44 1. 00 25. 47 1. 00 26. 84 1. 00 28. 30 1. 00 28. 21 1. 00 26. 82 1. 00 29. 86 1. 00 29. 86 1. 00 29. 50 1. 00 27. 80 1. 00 30. 32 1. 00 33. 05 1. 00 34. 99	A A A A A A A A A A A A A A A A A A A	CONCCCONCCCCONCCCC

	(Continued)									
ATOM	4704	CD (GLU	608	50.054	G. 4 66.482	62. 389	1.00 38.42	A	· C
ATOM	4705	0E1 (608	49. 197	66.454	63. 302	1.00 37.67	A	0
ATOM	4706	0E2 (608	51. 285	66. 435	62.625	1.00 40.64	A	0
ATOM	4707		GLU	608	50.606	63.891	60.012	1.00 32.76	A	C
ATOM	4708		GLU	608	49.889	63. 527 63. 270	60. 947 58. 836	1.00 33.47 1.00 31.32	A A	0 N
ATOM	4709		ALA	609	50. 643 49. 827	62.090	58. 595	1.00 31.32	A	Č
ATOM	4710		ALA ALA	609 609	49. 883	61.682	57. 123	1.00 28.50	A	č
ATOM ATOM	4711 4712		ALA ALA	609	50. 355	60.968	59. 472	1.00 28.30	A	č
ATOM	4713		ALA	609	49. 583	60. 274	60. 139	1.00 31.03	A	ŏ
ATOM	4714		ALA	610	51.674	60.803	59.479	1.00 29.26	A	Ň
ATOM	4715		ALA	610	52.310	59. 758	60. 274	1.00 28.48	A	C
ATOM	4716		ALA	610	53. 826	59.818	60.114	1.00 27.67	A	С
ATOM	4717		ALA	610	51.930	59.886	61.743	1.00 27.62	Α	С
ATOM	4718		ALA	610	51.556	58.904	62.379	1.00 28.43	Α	0
ATOM	4719		ARG	611	52.025	61.094	62.282	1.00 26.94	Α	N
ATOM -	4720	CA A	ARG	611	51.674	61.309	63.678	1.00 28.98	Α	C
ATOM	4721		ARG	611	51.812	62.787	64.042	1.00 28.96	A	C
ATOM	4722		ARG	611	53. 239	63. 291	64.032	1.00 29.26	A	C
ATOM	4723		ARG	611	53. 281	64. 799	64.187	1.00 29.92	A	C
ATOM	4724		ARG	611	54. 641	65. 322	64. 102	1.00 28.90	A	N .
ATOM	4725		ARG	611	54. 980	66. 384		1.00 29.97	A	C
ATOM	4726	NH1		611	54. 055	67.028	62.680	1.00 31.41	A	Ň N
ATOM	4727	NH2		611	56. 237	66. 802	63. 347	1.00 29.57	A	N C
ATOM	4728		ARG	611	50. 242	60.846	63. 923 64. 856	1.00 29.90 1.00 31.08	A A	0
ATOM	4729		ARG GLN	611 612	49. 983 49. 319	60. 084 61. 298	63. 076	1.00 31.08	A	N N
ATOM ATOM	4730 4731		GLN	612	47. 916	60. 922	63. 195	1.00 30.18	A	Č
ATOM	4732		GLN	612	47. 108	61.497	62. 035	1.00 30.42	A	Č
ATOM	4733		GLN	612	47. 112	63. 001	61.964	1.00 33.70	A	č
ATOM	4734		GLN	612	46. 446	63. 637	63. 162	1.00 34.91	A	č
ATOM	4735	0E1		612	45. 276	63. 379	63. 444	1.00 35.03	Ā	0
ATOM	4736	NE2		612	47. 188	64. 475	63.875	1.00 35.30	A	N
ATOM	4737		GLN .	612	47.740	59.405	63. 223	1.00 30.70	Α	С
ATOM	4738		GLN	612	46.993	58.878	64.049	1.00 31.56	Α	0
ATOM	4739	N]	PHE	613	48. 415	58.698	62.324	1.00 30.50	Α	N
ATOM	4740		PHE	613	48. 291	57. 248	62. 301	1.00 32.33	Α	С
ATOM	4741		PHE	613	49. 043	56.653	61.114	1.00 31.37	A	C C
ATOM	4742		PHE	613	48. 537	57.126	59. 787	1.00 30.49	A	C
ATOM	4743	CD1		613	47. 167	57. 171	59. 529	1.00 30.03	A	C
ATOM	4744	CD2		613	49. 423	57. 523	58. 793	1.00 28.11	A	C
ATOM	4745	CE1		613	46. 687	57.604	58.300	1.00 29.96	A	C C
ATOM	4746	CE2		613	48. 954	57. 959	57. 559	1.00 28.75	A	C C
ATOM	4747		PHE	613	47. 585	58.001	57. 309	1.00 28.70	A	C
ATOM	4748		PHE	613	48. 835	56.679	63.597	1.00 34.28 1.00 34.47	A A	C 0
ATOM	4749		PHE	613	48. 327	55. 677 57. 326	64. 107 64. 134	1.00 34.47	A A	N N
ATOM	4750		SER	614	49. 865	57. 326 56. 884	65.388	1.00 33.01	A	C
ATOM	4751 4752		SER SER	614 614	50. 454 51. 723		65.683	1.00 38.32	A	Č
ATOM	7106	CD	الزار	014	91.123	J1. U1 (00.000	1.00 00.00	11	J

					77.1	0 4	0.0			(Continued)
					F 1 (G. 4·	98			
ATOM	4753	0G	SER	614	52.686	57. 477	64.663	1.00 38.53	A	0
ATOM	4754	C	SER	614	49. 424	57.098	66. 494	1.00 39.76	A	C
ATOM	4755	0	SER	614	49. 283	56. 276	67. 398	1.00 41.47	A	0 N
ATOM	4756	N	LYS	615	48. 694	58. 204	66. 413 67. 400	1.00 40.51 1.00 41.32	A A	N C
ATOM	4757	CA	LYS LYS	615 615	47. 663 47. 047	58. 490 59. 870	67. 155	1.00 41.32	A	Č
ATOM ATOM	4758 4759	CB CG	LYS	615	47. 884	61.040	67. 642	1.00 44.59	A	č
ATOM	4760	CD	LYS	615	47.064	62. 330	67. 631	1.00 46.18	Ä	č
ATOM	4761	CE	LYS	615	47. 864	63. 511	68. 168	1.00 46.73	Ā	Č
ATOM	4762	NZ	LYS	615	48.314	63. 301	69.577	1.00 48.03	Α	N
ATOM	4763	C	LYS	615	46.552	57.441	67.347	1.00 40.86	Α	C
ATOM	4764	Ō	LYS	615	45.794	57. 285	68.303	1.00 41.94	Α	0
ATOM	4765	N	MET	616	46.456	56.724	66.230	1.00 39.78	Α	N
ATOM	4766	CA	MET	616	45.418	55.712	66.065	1.00 37.88	A	C
ATOM	4767	CB	MET	616	45. 246	55. 374	64.578	1.00 37.42	A	C
ATOM	4768	CG	MET	616	44. 673	56. 532	63.768	1.00 35.95	A	C
ATOM	4769	SD	MET	616	44. 195	56. 101	62.079	1.00 35.73	A	S
ATOM	4770	CE	MET	616	43. 946	57. 730	61.385	1.00 34.06	A	C
ATOM	4771	C	MET	616	45.654	54. 447	66.885	1.00 36.90	A	C 0
ATOM	4772	0	MET	616	44. 908	53.473	66. 772 67. 698	1.00 37.22 1.00 35.15	A A	N N
ATOM	4773	N CA	GLY	617 617	46. 706 47. 013	54. 469 53. 355	68. 578	1.00 33.13	A	C
ATOM	4774 4775	CA C	GLY GLY	617	47. 445	51.995	68. 065	1.00 32.74	A	Č
ATOM ATOM	4776	0	GLY	61.7	47. 806	51.143	68. 872	1.00 33.71	A	ŏ
ATOM	4777	N	PHE	618	47. 409	51.751	66. 761	1.00 32.52	Ä	Ň
ATOM	4778	CA	PHE	618	47. 841	50.447	66. 262	1.00 31.36	Ä	Č
ATOM	4779	CB	PHE	618	46. 701	49.759	65.496	1.00 31.10	Α	С
ATOM	4780	ĊĠ	PHE	618	46.047	50.624	64.457	1.00 31.61	Α	С
ATOM	4781		PHE	618	46.743	51.025	63.322	1.00 31.30	Α	C
ATOM	4782		PHE	618	44. 724	51.027	64.607	1.00 30.93	Α	С
ATOM	4783		PHE	618	46. 129	51.815	62.349	1.00 31.53	A	C
ATOM	4784		PHE	618	44. 104	51.814	63.642	1.00 30.94	A	C
ATOM	4785	CZ	PHE	618	44. 808	52. 209	62.509	1.00 29.86	A	C
ATOM	4786	C	PHE	618	49. 109	50. 521	65. 404	1.00 30.95	A	C
ATOM	4787	0	PHE	618	49. 303	49.735	64. 477	1.00 30.95	A	0
ATOM	4788	N	VAL	619	49. 982	51.465	65. 732 64. 996	1.00 30.23 1.00 29.99	A	N C
ATOM	4789	CA	VAL VAL	619 619	51.226	51.627 52.928	64. 147	1.00 29.39	A A	C C
ATOM ATOM	4790 4791	CB	VAL	619	51. 226 52. 632	53. 200	63. 617	1.00 28.74	A	Č
ATOM	4792		VAL	619	50. 248	52. 804	62. 994	1.00 26.48	A	č
ATOM	4793	C	VAL	619	52. 425	51.673	65. 931	1.00 29.66	Ä	č
ATOM	4794	ŏ	VAL	619	52. 400	52. 342	66. 962	1.00 30.05	Ä	ŏ
ATOM	4795	Ň	ASP	620	53. 475	50.954	65. 561	1.00 29.84	Ä	Ň
ATOM	4796	CA	ASP	620	54. 695	50.932	66.347	1.00 29.07	Α	С
ATOM	4797	CB	ASP	620	55. 563	49.748	65.924	1.00 27.94	Α	C
ATOM	4798	CG	ASP	620	56. 789	49. 587	66.794	1.00 27.02	Α	С
ATOM	4799	0D1		620	57. 191	50. 580	67.439	1.00 26.38	A	0
ATOM	4800		ASP	620	57. 358	48. 473	66. 818	1.00 25.22	Ą	0
ATOM	4801	C	ASP	620	55. 408	52. 243	66. 039	1.00 30.30	A	C

					FΙ	G. 4	- 9 9			(Continued)
ATOM ATOM ATOM ATOM ATOM	4802 4803 4804 4805 4806	N CA CB	ASP ASN ASN ASN ASN	620 621 621 621 621	56. 009 55. 330 55. 962 55. 761 56. 420	52. 398 53. 196 54. 492 55. 376 54. 804	64. 979 66. 958 66. 746 67. 975 69. 214	1.00 29.95 1.00 33.01 1.00 35.15 1.00 38.29 1.00 43.03	A A A A	O N C C C
ATOM ATOM ATOM	4807 4808	OD1 ND2	ASN ASN	621 621	57. 648 55. 606	54. 821 54. 280 54. 370	69. 346 70. 130	1.00 44.79 1.00 45.61	A A	O N
ATOM ATOM	4809 4810 4811	O N	ASN ASN LYS	621 621 622	57. 453 58. 083 58. 016	55. 330 53. 186	66. 441 66. 004 66. 660	1. 00 35. 20 1. 00 34. 67 1. 00 36. 30	A A A	C 0 N
ATOM ATOM ATOM	4812 4813 4814	CB CG	LYS LYS LYS	622 622 622	60. 030 60. 148	52. 977 52. 027 52. 611	66. 418 67. 464 68. 866	1. 00 35. 70 1. 00 37. 42 1. 00 39. 14	A A A	C C C
ATOM ATOM ATOM	4815 4816 4817	CE NZ	LYS LYS LYS	622 622 622	60. 763 60. 839 61. 516	51. 584 52. 077 51. 077	69. 804 71. 240 72. 123	1. 00 43. 05 1. 00 45. 27 1. 00 45. 73	A A A	C C N
ATOM ATOM ATOM	4818 4819 4820	O N	LYS LYS ARG	622 622 623	59. 762 60. 896 58. 783	52. 445 52. 572 51. 846	65. 036 64. 571 64. 374	1. 00 34. 38 1. 00 35. 67 1. 00 31. 86	A A A	C O N
ATOM ATOM ATOM	4821 4822 4823	CB CG	ARG ARG ARG	623 623 623	59. 030 58. 821 59. 767	51. 308 49. 791 49. 071	63. 046 63. 058 64. 009	1.00 29.60 1.00 29.94 1.00 32.12	A A A	C C C
ATOM ATOM ATOM	4824 4825 4826	NE CZ	ARG ARG ARG	623 623 623	59. 117 59. 247 58. 457	47. 832 46. 663 45. 601	64. 614 63. 758 63. 833	1.00 33.42 1.00 34.25 1.00 34.36	A A A	C N C
ATOM ATOM ATOM	4827 4828 4829		ARG ARG	623 623 623	57. 476 58. 655 58. 179	45. 572 44. 571 51. 957	64. 725 63. 021 61. 962	1.00 35.41 1.00 33.15 1.00 27.66	A A A	N N C
ATOM ATOM ATOM	4830 4831 4832	N CA	ARG ILE ILE	623 624 624	57. 315 58. 425 57. 708	51. 313 53. 241 53. 977	61. 363 61. 720 60. 685	1.00 27.44 1.00 25.16 1.00 24.70	A A A	0 - N C
ATOM ATOM ATOM	4833 4834 4835	CG2 CG1	ILE	624 624 624	57. 114 56. 391 56. 136	55. 298 56. 025 55. 021	61. 224 60. 107 62. 371	1.00 24.52 1.00 23.47 1.00 24.01	A A A	C C C
ATOM ATOM ATOM	4836 4837 4838		ILE ILE	624 624 624	55. 473 58. 667 59. 651	55.034	59.709	1.00 19.15 1.00 24.37 1.00 23.38	A A A	C C O
ATOM ATOM ATOM	4839 4840 4841	CA CB	ALA ALA ALA	625 625 625	58. 384 59. 213 59. 650	53. 768 54. 014 52. 693	58. 356 57. 189 56. 579	1.00 22.58 1.00 21.00 1.00 20.21	A A A	N C C
ATOM ATOM ATOM	4842 4843 4844	0 N	ALA ALA ILE	625 625 626	58. 430 57. 209 59. 135	54. 833 54. 966 55. 385	56. 168 56. 275 55. 185	1.00 21.28 1.00 21.90 1.00 19.63	A A A	C O N
ATOM ATOM ATOM	4845 4846 4847	CB CG2		626 626 626	58. 502 58. 589 60. 032	56. 178 57. 699 58. 103	54. 137 54. 446 54. 694	1.00 18.63 1.00 18.98 1.00 18.36	A A A	C C C
ATOM ATOM ATOM	4848 4849 4850	CG1 CD1 C		626 626 626	57. 973 57. 872 59. 185	58. 501 59. 991 55. 882	53. 296 53. 562 52. 809	1.00 19.11 1.00 18.34 1.00 17.48	A A A	C C C

					FIG	. 4 -	100	,		(Cont	tinued)
ATOM ATOM ATOM ATOM ATOM ATOM	4852 4853 4854 4855 4856	N CA CB CG CD2		626 627 627 627 627 627	60. 380 58. 425 58. 998 59. 190 58. 096 58. 139	55. 619 55. 893 55. 622 54. 118 53. 441 53. 055 52. 425	52. 776 51. 719 50. 409 50. 206 49. 427 48. 044 47. 749	1.00 17.10 1.00 17.62 1.00 17.62 1.00 16.80 1.00 18.70 1.00 17.58 1.00 17.70	A A A A A	O N C C C C	
ATOM ATOM ATOM ATOM ATOM ATOM	4858 4859 4860 4861 4862 4863	CZ2 CZ3 CH2	TRP TRP TRP TRP TRP TRP	627 627 627 627 627 627 627 627	56. 912 59. 095 56. 879 56. 163 56. 617 58. 801 57. 575 58. 157	52. 425 53. 179 53. 047 52. 435 51. 916 52. 673 52. 048 56. 191	47. 028 49. 895 48. 896 46. 480 45. 769 45. 507 49. 275	1. 00 15. 10 1. 00 18. 68 1. 00 18. 72 1. 00 16. 42 1. 00 14. 48 1. 00 14. 63 1. 00 18. 48	A A A A A A	C C N C C C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4864 4865 4866 4867 4868 4869 4870 4871	O N CA C	TRP TRP GLY GLY GLY TRP TRP	627 628 628 628 628 628 629	56. 934 58. 829 58. 140 58. 986 60. 212 58. 312 58. 945	56. 280 56. 579 57. 146 57. 163 57. 065 57. 300 57. 322	49. 381 48. 193 47. 049 45. 787 45. 833 44. 654 43. 343	1. 00 18. 15 1. 00 18. 70 1. 00 18. 30 1. 00 18. 36 1. 00 19. 07 1. 00 17. 25 1. 00 15. 27	A A A A A A	0 N C C O N C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4872 4873 4874 4875 4876 4877 4878	CB CG CD2 CE2 CE3 CD1 NE1	TRP TRP TRP TRP TRP TRP	629 629 629 629 629 629 629	58. 306 59. 131 59. 512 60. 243 59. 312 59. 635 60. 299	56. 214 55. 698 54. 335 54. 310 53. 135 56. 422	42. 494 41. 357 41. 122 39. 914 41. 818 40. 313 39. 443	1.00 10.48 1.00 10.84 1.00 9.02 1.00 10.87 1.00 9.31 1.00 10.72 1.00 10.74	A A A A A	C C C C C N	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4879 4880 4881 4882 4883 4884 4885	CZ2 CZ3	TRP TRP TRP TRP TRP SER SER	629 629 629 629 629 630	60. 779 59. 842 60. 571 58. 671 57. 622 59. 612 59. 453	53. 126 51. 959 51. 965 58. 722 59. 300 59. 269	39. 379 41. 295 40. 080 42. 753 43. 012 41. 983 41. 383	1.00 12.40 1.00 11.95 1.00 13.29 1.00 15.91 1.00 15.58 1.00 16.99 1.00 16.78	A A A A A	C C C O N C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4886 4887 4888 4889 4890 4891 4892		SER SER SER SER TYR TYR TYR	630 630 630 630 631 631 631	58. 258 58. 531 59. 234 60. 076 58. 093 57. 737 56. 380	60. 644 59. 987 61. 656 61. 856 62. 335 63. 362	39. 198 42. 450 43. 321 42. 368 43. 335	1. 00 18. 65 1. 00 22. 38 1. 00 16. 69 1. 00 17. 90 1. 00 17. 21 1. 00 15. 51 1. 00 17. 16	A A A A A	C O C O N C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4893 4894 4895 4896 4897 4898 4899	CG CD1 CE1 CD2	TYR TYR TYR TYR TYR TYR TYR TYR	631 631 631 631 631 631	56. 161 55. 947 55. 741 56. 168 55. 963 55. 748 55. 520	65. 353 65. 550 66. 826 66. 470 67. 751 67. 918	43. 545 44. 909 45. 429 42. 714 43. 226 44. 580	1.00 19.30 1.00 19.21	A A A A A A	C C C C C O	

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										(Continued)
					FIC	G. 4-	101			(Continued)
ATOM	4900	C	TYR	631	57. 672	62.632	44.668	1.00 15.27	A	С
ATOM	4901	0	TYR	631	57.946	63. 201	45. 731	1.00 13.23	A	0
ATOM	4902	N	GLY	632	57. 324	61.350	44. 592	1.00 14.83	A	N
ATOM	4903	CA	GLY	632	57. 266	60. 529	45. 783	1.00 15.04	A	C
ATOM ATOM	4904 4905	C 0	GLY GLY	632 632	58. 653 58. 816	60. 477 60. 652	46. 394 47. 596	1.00 14.53 1.00 13.85	A A	C 0
ATOM	4906	N	GLY	633	59. 655	60. 246	47. 550	1.00 15.63	A	N N
ATOM	4907	CA	GLY	633	61.030	60. 185	46.014	1.00 14.69	A	Č
ATOM	4908	C	GLY	633	61.500	61.513	46. 576	1.00 15.25	Ä	č
ATOM	4909	0	GLY	633	62.251	61.561	47. 555	1.00 16.82	Ā	0
ATOM	4910	N	TYR	634	61.058	62.598	45.954	1.00 13.67	Α	N
ATOM	4911	CA	TYR	634	61.418	63.940	46.398	1.00 13.29	Α	C
ATOM	4912	CB	TYR	634	60.901	64. 964	45. 397	1.00 11.67	A	C
ATOM	4913	CG	TYR	634	60.914	66.382	45.904	1.00 12.54	A	C
ATOM	4914		TYR	634	62.112	67.069	46.072	1.00 13.46	A	C
ATOM ATOM	4915 4916		TYR TYR	634 634	62. 125 59. 723	68. 398 67. 057	46. 484 46. 173	1.00 13.37 1.00 11.38	A	C C
ATOM	4917		TYR	634	59. 727	68. 383	46. 586	1.00 11.36	A A	Č
ATOM	4918	CZ	TYR	634	60. 933	69.049	46. 734	1.00 12.83	A	Č
ATOM	4919	OH	TYR	634	60. 957	70. 375	47. 091	1.00 12.97	A	ŏ
ATOM	4920	C	TYR	634	60.829	64. 240	47.778	1.00 14.36	Ā	Č
ATOM	4921	0	TYR	634	61.524	64.721	48.672	1.00 16.28	A	0
ATOM	4922	N	VAL	635	59. 542	63. 968	47. 949	1.00 14.99	Α	N
ATOM	4923	CA	VAL	635	58. 899	64. 218	49. 231	1.00 15.44	A	C
ATOM	4924	CB	VAL	635	57. 364	64. 025	49. 135	1.00 15.15	A	C
ATOM ATOM	4925 4926	CG2	VAL	635	56.743	63. 988	50. 524	1.00 14.56	A	C
ATOM	4927	C	VAL	635 635	56. 758 59. 486	65. 167 63. 296	48. 326 50. 294	1.00 12.62 1.00 16.48	. A	C C
ATOM	4928	Ö	VAL	635	59. 681	63. 711	50. 294	1.00 16.48	A A	0
ATOM	4929	Ň	THR	636	59.779	62. 054	49. 917	1.00 16.16	A	N N
ATOM	4930	CA	THR	636	60.368	61.098	50. 855	1.00 18.40	Ä	Č
ATOM	4931	CB	THR	636	60.701	59.746	50.175	1.00 18.30	Ä	č
ATOM	4932	0G1	THR	636	59.504	59.130	49.696	1.00 20.57	Α	0
ATOM	4933	CG2		636	61.362	58.807	51.157	1.00 20.48	Α	C
ATOM	4934	C	THR	636	61.676	61.676	51.396	1.00 19.91	A	С
ATOM	4935	0	THR	636	61.914	61.696	52. 609	1.00 19.58	A	0
ATOM ATOM	4936	N	SER	637	62. 524	62. 141	50. 483	1.00 19.89	A	N
ATOM	4937 4938	CA CB	SER SER	637 637	63. 804 64. 599	62. 711 63. 086	50. 862	1.00 20.30	A	C
ATOM	4939	OG	SER	637	64. 823	61.952	49. 614 48. 800	1.00 19.17 1.00 19.07	A	C
ATOM	4940	C	SER	637	63. 615	63. 938	51.749	1.00 13.07	. А А	0 C
ATOM	4941	ŏ	SER	637	64. 235	64.049	52. 812	1.00 21.01	A	. 0
ATOM	4942	Ň	MET	638	62.760	64. 855	51.309	1.00 21.06	A	N N
ATOM	4943	CA	MET	638	62.490	66.074	52.066	1.00 21.87	A	Ċ
ATOM	4944		MET	638	61.417	66.895	51.354	1.00 20.36	Ä	C
ATOM	4945		MET	638	61.876	67.465	50.032	1.00 21.23	Α	С
ATOM	4946		MET	638	63.069	68. 787	50. 261	1.00 21.33	A	S
ATOM	4947		MET	638	62.006	70. 229	50. 125	1.00 19.31	A	C
ATOM	4948	С	MET	638	62. 039	65. 748	53. 494	1.00 21.51	A	C

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										(Continued)
					FIG.	. 4 -	102			(00111111111111111111111111111111111111
ATOM	4949	0	MET	638	62. 511	66. 351	54. 472	1.00 19.64	A	0
ATOM	4950	N	VAL	639		64. 798	53.600	1.00 19.63	A	N
ATOM	4951	CA	VAL	639		64. 372	54.891	1.00 20.04	A	C
ATOM	4952	CB	VAL	639		63. 287	54.746	1.00 20.08	Α	C
ATOM	4953	CG1	VAL	639	59. 201	62.688	56. 112	1.00 20.55	Α	C
ATOM	4954	CG2	VAL	639	58. 27 5	63. 879	54. 108	1.00 17.95	Α	С
ATOM	4955	C	VAL	639	61.758	63. 793	55.692	1.00 20.25	Α	С
ATOM	4956	0	VAL	639	61.986	64. 185	56.831	1.00 23.11	A	0
ATOM	4957	N	LEU	640		62.864	55.088	1.00 20.83	Α	N
ATOM	4958	CA	LEU	640		62.225	55. 765	1.00 22.08	Α	C
ATOM	4959	CB	LEU	640		61. 179	54.855	1.00 22.31	Α	C
ATOM	4960	CG	LEU	640		59. 939	54. 570	1.00 21.31	A	C
ATOM	4961		LEU	640		59. 041	53.611	1.00 22.16	A	C
ATOM	4962		LEU	640		59. 205	55.863	1.00 22.25	A	C
ATOM	4963	C	LEU	640	64.675	63. 212	56. 239	1.00 23.38	Α	C
ATOM	4964	0	LEU	640		62.922	57. 182	1.00 22.99	A	0
ATOM	4965	N	GLY	641		64. 374	55. 592	1.00 23.16	A	N
ATOM	4966	CA	GLY	641		65. 368	55. 972	1.00 23.10	A	C
ATOM	4967	C	GLY	641		66. 555	56. 721	1.00 23.73	A	C
ATOM	4968	0	GLY	641		67. 609	56. 802	1.00 23.94	A	0
ATOM	4969	N	SER	642		66. 393	57. 278	1.00 22.74	A	N
ATOM	4970	CA	SER	642		67. 484	58.002	1.00 20.76	A	C
ATOM	4971	CB	SER	642		67. 370	57. 883	1.00 19.77	A	C
ATOM	4972	0G	SER	642		66. 213	58. 546	1.00 17.97	A	0
ATOM	4973	C	SER	642		67.488	59. 471	1.00 21.73	A	C
ATOM	4974	0	SER	642		68.519	60.140	1.00 21.40	A	0
ATOM	4975	N	GLY	643		66.327	59.967	1.00 22.24	A	N
ATOM	4976	CA	GLY	643		66.213	61.350	1.00 22.64	A	C
ATOM	4977	C	GLY	643		65.944	62.314	1.00 23.74	A	C
ATOM ATOM	4978 4979	O N	GLY SER	643 644		66. 064 65. 573	63. 528 61. 786	1.00 25.32 1.00 23.53	A	0 N
ATOM	4979	CA	SER	644		65. 301	62.616	1.00 23.38	A	N C
ATOM	4981	CB	SER	644		64. 995	61.742	1.00 23.36	A	Č
ATOM	4982	OG	SER	644		63. 666	61.247	1.00 24.19	A A	0
ATOM	4983	C	SER	644		64. 129	63. 559	1. 00 24. 43	A	C
ATOM	4984	Õ	SER	644		53. 961	64. 536	1.00 23.18	A	Ö
ATOM	4985	N	GLY	645		33. 307	63. 258	1. 00 24. 28	Ä	N N
ATOM	4986	CA	GLY	645		52. 166	64. 107	1.00 24.80	A	Č
ATOM	4987	C	GLY	645		51. 175	64. 114	1.00 24.80	A	č
ATOM	4988	ŏ	GLY	645		50. 248	64. 920	1.00 27.93	A	ŏ
ATOM	4989	N	VAL	646		31. 357	63. 207	1.00 23.98	Ä	N
ATOM	4990	CA	VAL	646		50.474	63. 121	1.00 23.30	A	Ĉ
ATOM	4991	CB	VAL	646		51. 207	62.473	1.00 -24.36	A	č
ATOM	4992	CG1		646		50. 230	62. 215	1.00 24.00	A	č
ATOM	4993		VAL	646		32. 351	63. 381	1.00 24.11	Ä	č
ATOM	4994	C	VAL	646		59. 202	62.327	1.00 21.28	A	č
ATOM	4995	Ŏ	VAL	646		58. 128	62.690	1.00 21.25	Ä	Ŏ
ATOM	4996	Ň	PHE	647		59. 326	61. 239	1.00 21.00	Ä	N
ATOM	4997	CA	PHE	647		8. 182	60. 380	1.00 18.33	Ä	Ĉ
							-	· -		

				EIC 4-109	(Continued)
				FIG. 4-103	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4998 4999 5000 5001 5002 5003 5004 5005 5006 5007 5008	CB PHE CG PHE CD1 PHE CD2 PHE CE1 PHE CE2 PHE C PHE C PHE N LYS CA LYS CB LYS	647 647 647 647 647 647 647 647 648 648	60. 497 58. 615 58. 924 1. 00 15. 79 A 59. 142 59. 131 58. 551 1. 00 16. 11 A 58. 138 58. 258 58. 152 1. 00 15. 39 A 58. 841 60. 479 58. 680 1. 00 14. 43 A 56. 855 58. 722 57. 894 1. 00 13. 82 A 57. 562 60. 943 58. 423 1. 00 15. 28 A 56. 568 60. 061 58. 031 1. 00 13. 75 A 61. 944 57. 555 60. 663 1. 00 18. 46 A 62. 943 58. 250 60. 825 1. 00 20. 84 A 61. 958 56. 232 60. 722 1. 00 17. 11 A 63. 165 55. 480 60. 996 1. 00 19. 06 A 62. 789 54. 105 61. 545 1. 00 17. 86 A	C C C C C C C C C C C C C C C C C C C
ATOM	5010	CG LYS	648	63.961 53.242 61.955 1.00 17.94 A	C
ATOM ATOM	5011 5012	CD LYS CE LYS	648 648	63.484 51.869 62.405 1.00 19.57 A 64.594 51.083 63.095 1.00 19.22 A	
ATOM ATOM	5013 5014	NZ LYS C LYS	648	65. 757 50. 894 62. 204 1. 00 20. 59 A	N
ATOM	5015	0 LYS	648 648	64.025 55.314 59.747 1.00 21.47 A 65.251 55.379 59.815 1.00 23.13 A	
ATOM ATOM	5016 5017	N CYS CA CYS	649 649	63. 376 55. 094 58. 610 1. 00 22. 38 A	N
ATOM	5018	C CYS	649	64. 077 54. 898 57. 353 1. 00 24. 23 A 63. 156 55. 237 56. 181 1. 00 24. 09 A	
ATOM	5019	0 CYS	649	61.939 55.319 56.342 1.00 23.94 A	0
ATOM ATOM	5020 5021	CB CYS	649 649	64. 527 53. 447 57. 237 1. 00 27. 68 A 63. 130 52. 287 57. 313 1. 00 32. 05 A	
ATOM	5022	N GLY	650	63. 130 52. 287 57. 313 1. 00 32. 05 A 63. 746 55. 426 55. 004 1. 00 21. 50 A	
ATOM	5023	CA GLY	650	62. 961 55. 757 53. 834 1. 00 21. 04 A	
ATOM ATOM	5024 5025	C GLY O GLY	650 650	63. 649 55. 384 52. 535 1. 00 21. 13 A	
ATOM	5026	N ILE	651	64. 874 55. 333 52. 474 1. 00 21. 62 A 62. 857 55. 124 51. 499 1. 00 19. 35 A	
ATOM	5027	CA ILE	651	63. 388 54. 753 50. 195 1. 00 19. 18 A	
ATOM	5028	CB ILE	651	62. 896 53. 352 49. 758 1. 00 19. 03 A	C
ATOM ATOM	5029 5030	CG2 ILE CG1 ILE	651 651	63. 601 52. 933 48. 481 1. 00 17. 31 A 63. 173 52. 326 50. 853 1. 00 19. 60 A	C
ATOM	5031	CD1 ILE	651	63. 173 52. 326 50. 853 1. 00 19. 60 A 62. 827 50. 901 50. 456 1. 00 18. 48 A	-
ATOM	5032	C ILE	651	62.953 55.749 49.120 1.00 19.53 A	č
ATOM ATOM	5033 5034	0 ILE N ALA	651	61. 758 56. 015 48. 949 1. 00 19. 77 A	0
ATOM	5035	N ALA CA ALA	652 652	63. 925 56. 292 48. 393 1. 00 18. 34 A 63. 633 57. 240 47. 324 1. 00 15. 69 A	N C
ATOM	5036	CB ALA	652	63. 633 57. 240 47. 324 1. 00 15. 69 A 64. 323 58. 574 47. 594 1. 00 14. 05 A	C C
ATOM	5037	C ALA	652	64.107 56.662 45.996 1.00 14.98 A	č
ATOM ATOM	5038 5039	O ALA N VAL	652	65. 288 56. 367 45. 827 1. 00 14. 12 A	0
ATOM	5040	CA VAL	653 653	63. 175 56. 487 45. 064 1. 00 14. 68 A 63. 492 55. 963 43. 738 1. 00 14. 84 A	N C
ATOM	5041	CB VAL	653	62.582 54.754 43.366 1.00 17.41 A	C
ATOM	5042	CG1 VAL	653	62. 865 54. 291 41. 932 1. 00 14. 95 A	C
ATOM ATOM	5043 5044	CG2 VAL C VAL	653 653	62. 806 53. 607 44. 352 1. 00 18. 10 A	C
ATOM	5045	0 VAL	653	63. 292 57. 063 42. 694 1. 00 13. 22 A 62. 224 57. 669 42. 620 1. 00 11. 12 A	C 0
ATOM	5046	N ALA	654	64. 331 57. 317 41. 901 1. 00 12. 68 A	N

										(Contin	ued)
					FIG	3.4-	104				
ATOM	5047	CA	ALA	654	64. 289	58. 327	40.845	1.00 10.68	A	С	
ATOM	5048	CB	ALA	654	63. 513	57. 790	39.650	1.00 7.27	A	C	
ATOM	5049	C	ALA	654	63. 653	59.607	41.352	1.00 10.02	A	C	
ATOM	5050	0	ALA	654	62.687	60. 103	40. 787	1.00 13.18	A	0 N	
MOTA	5051		PRO	655 655	64. 208	60.179	42.420	1.00 10.68 1.00 8.01	A	N C	
ATOM ATOM	5052 5053		PRO PRO	655 655	65. 319 63. 643	59. 696 61. 408	43. 262 42. 971	1.00 8.01 1.00 10.40	A A	C C	
ATOM	5054	CB	PRO	655	64. 092	61.344	44. 422	1.00 10.40	A.	Č	
ATOM	5055		PRO	655	65. 476	60. 822	44. 277	1.00 6.23	Ä	č	
ATOM	5056	Č	PRO	655	64.090	62. 714	42. 327	1.00 12.92	Ā	Č	
ATOM	5057	0	PRO	655	65.166	62.793	41.717	1.00 13.38	Α	0	
ATOM	5058	N	VAL	656	63. 245	63. 735	42.454	1.00 12.39	Α	N	
ATOM	5059	CA	VAL	656	63. 612	65.065	41.999	1.00 12.85	A	C	
ATOM	5060	CB	VAL	656	62. 373	65. 946	41.769	1.00 11.42	A	C	
ATOM	5061		VAL	656	62. 781	67.416	41.645	1.00 10.52	A	C	
ATOM	5062	CG2		656	61.661	65. 500	40.510	1.00 10.18	A	C	
ATOM ATOM	5063 5064	C 0	VAL VAL	656 656	64. 382 64. 038	65. 560 65. 188	43. 236 44. 355	1.00 13.79 1.00 14.63	A A	C 0	
ATOM	5065	N	SER	657	65. 419	66. 372	43.066	1.00 14.03	A	N N	
ATOM	5066	CA	SER	657	66. 174	66. 831	44. 238	1.00 14.21	A	Č	
ATOM	5067	CB	SER	657	67. 589	66. 231	44. 231	1.00 15.67	Ä	č	
ATOM	5068	0G	SER	657	68. 385	66.819	43.213	1.00 15.19	Ā	Ŏ	
ATOM	5069	C	SER	657	66. 286	68.343	44.320	1.00 14.77	A	C	
ATOM	5070	0	SER	657	66. 387	68. 912	45.406	1.00 14.39	Α	0	
ATOM	5071	N	ARG	658	66. 269	68. 978	43. 158	1.00 15.05	A	N	
ATOM	5072		ARG	658	66. 388	70. 423	43.038	1.00 16.33	A	C	•
ATOM	5073		ARG	658	67. 845	70. 787	42.747	1.00 20.44	A	C	
ATOM ATOM	5074 5075		ARG ARG	658 658	68. 142 69. 543	72. 274 72. 450	42.582 42.025	1.00 24.34 1.00 25.38	A	C C	
ATOM	5076		ARG	658	69. 905	73. 838	41.757	1.00 25.30	A A	N N	
ATOM	5077	CZ	ARG	658	70. 353	74. 683	42.676	1.00 28.34	A	Č	
ATOM	5078		ARG	658	70. 491	74. 288	43. 935	1.00 28.23	A	Ň	
ATOM	5079	NH2		658	70.690	75.916	42.329	1.00 29.55	A	N	
ATOM	5080	C	ARG	658	65.515	70.775	41.850	1.00 15.87	Α	С	
ATOM	5081	0	ARG	658	65. 752	70. 288	40. 735	1.00 16.75	Α	0	
ATOM	5082	N	TRP	659	64. 514	71.616	42.073	1.00 13.52	A	N	
ATOM	5083		TRP	659	63. 603	71.967	40. 999	1.00 13.69	A	C	
ATOM	5084	CB	TRP	659	62. 465	72. 823	41.550	1.00 13.63	A	C	
ATOM ATOM	5085 5086	CG CD2	TRP	659 659	61. 504 60. 690	71. 963 70. 898	42. 341 41. 829	1.00 17.48 1.00 16.63	A	C C	
ATOM	5087	CE2		659	60. 027	70. 313	42. 927	1.00 10.03	A A	C	
ATOM	5088	CE3		659	60.460	70. 382	40. 547	1.00 16.00	A	Č	
ATOM	5089	CD1		659	61.300	71.980	43.692	1.00 17.21	A	Č	
ATOM	5090	NE1		659	60.418	70.993	44.050	1.00 17.37	Ä	Ň	
ATOM	5091	CZ2	TRP	659	59. 145	69. 233	42.785	1.00 21.55	A	Ċ	
ATOM	5092	CZ3		659	59. 584	69. 311	40.403	1.00 18.00	Α	C	
ATOM	5093	CH2		659	58. 937	68. 746	41.516	1.00 20.15	A	C	
ATOM	5094		TRP	659	64. 219	72. 580	39. 748	1.00 13.15	A	C	
ATOM	5095	0	TRP	659	63. 643	72. 503	38. 670	1.00 11.17	A	0	

ATOM 5096 N GLU 660 65.400 73.163 39.871 1.00 14.12 A N ATOM 5097 CA GLU 660 66.042 73.725 38.697 1.00 15.96 A C ATOM 5098 CB GLU 660 67.147 74.704 39.108 1.00 16.83 A C ATOM 5099 CG GLU 660 66.548 76.001 39.626 1.00 19.65 A C ATOM 5100 CD GLU 660 67.535 76.901 40.313 1.00 22.71 A C ATOM 5101 0E1 GLU 660 67.527 76.907 41.561 1.00 23.59 A O ATOM 5102 0E2 GLU 660 67.527 76.907 41.561 1.00 23.59 A O ATOM 5103 C GLU 660 67.527 76.907 41.561 1.00 23.59 A O ATOM 5104 0 GLU 660 67.507 72.635 37.777 1.00 15.29 A C ATOM 5105 N TYR 661 66.539 71.383 38.233 1.00 14.54 A N ATOM 5106 CA TYR 661 67.003 70.269 37.399 1.00 14.57 A C ATOM 5107 CB TYR 661 67.642 69.154 38.230 1.00 14.57 A C ATOM 5109 CD1 TYR 661 69.743 70.531 38.655 1.00 13.37 A C ATOM 5110 CE1 TYR 661 69.743 70.531 38.655 1.00 13.37 A C ATOM 5110 CE1 TYR 661 69.743 70.531 38.655 1.00 13.37 A C ATOM 5111 CD2 TYR 661 69.199 68.765 40.166 1.00 16.03 A C ATOM 5112 CE2 TYR 661 70.388 70.805 39.390 1.00 12.74 A C ATOM 5112 CE2 TYR 661 70.389 70.805 39.390 1.00 12.74 A C ATOM 5112 CE2 TYR 661 70.386 70.252 41.267 1.00 8.43 A O ATOM 5114 CD2 TYR 661 69.199 68.765 40.166 1.00 16.03 A C ATOM 5114 CD2 TYR 661 70.388 70.805 39.390 1.00 12.74 A C ATOM 5114 CD2 TYR 661 69.199 68.765 40.166 1.00 16.03 A C ATOM 5114 CD2 TYR 661 67.038 70.269 37.366 80.27 40.898 1.00 13.47 A C ATOM 5114 CD2 TYR 661 67.048 69.099 68.765 40.166 1.00 16.03 A C ATOM 5114 CD2 TYR 661 66.077 68.854 35.675 1.00 13.47 A C ATOM 5115 C TYR 661 66.077 68.854 35.675 1.00 13.47 A C ATOM 5116 O TYR 661 66.077 68.854 35.675 1.00 13.28 A N ATOM 5116 O TYR 662 64.602 69.963 36.984 1.00 13.28 A N ATOM 5118 CA TYR 662 63.445 69.390 36.308 1.00 14.01 A C ATOM 5119 CB TYR 662 64.602 69.963 36.802 1.00 15.74 A C ATOM 5119 CB TYR 662 64.602 69.963 36.802 1.00 14.50 A C ATOM 5120 CG TYR 662 63.445 69.390 36.308 1.00 14.01 A C ATOM 5120 CG TYR 662 63.445 69.390 36.802 1.00 15.74 A C ATOM 5120 CG TYR 662 63.445 69.390 36.802 1.00 14.50 A C ATOM 5120 CG TYR 662 63.445 69.390 36.802 1.00 14.99 A C
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ATOM 5098 CB GLU 660 67. 147 74. 704 39. 108 1. 00 16. 83 A C ATOM 5099 CG GLU 660 66. 548 76. 001 39. 626 1. 00 19. 65 A C ATOM 5100 CD GLU 660 67. 535 76. 901 40. 313 1. 00 22. 71 A C ATOM 5101 0E1 GLU 660 68. 310 77. 600 39. 617 1. 00 25. 18 A O ATOM 5102 0E2 GLU 660 67. 527 76. 907 41. 561 1. 00 25. 18 A O ATOM 5103 C GLU 660 66. 577 72. 635 37. 777 1. 00 15. 29 A C ATOM 5104 0 GLU 660 66. 577 72. 635 37. 777 1. 00 15. 29 A C ATOM 5105 N TYR 661 66. 539 71. 383 38. 233 1. 00 14. 54 A N ATOM 5106 CA TYR 661 67. 003 70. 269 37. 399 1. 00 14. 57 A C ATOM 5107 CB TYR 661 67. 642 69. 154 38. 230 1. 00 13. 59 A C ATOM 5109 CD1 TYR 661 69. 743 70. 531 38. 655 1. 00 13. 37 A C ATOM 5110 CE1 TYR 661 69. 199 68. 765 40. 166 1. 00 16. 63 A C ATOM 5112 CE2 TYR 661 70. 889 70. 805 39. 390 1. 00 12. 74 A C ATOM 5112 CE2 TYR 661 70. 338 69. 027 40. 898 1. 00 16. 63 A C ATOM 5113 CZ TYR 661 72. 322 70. 252 41. 267 1. 00 8. 43 A O ATOM 5115 C TYR 661 66. 5842 69. 637 36. 608 1. 00 15. 74 A C ATOM 5116 O TYR 661 66. 5842 69. 637 36. 608 1. 00 13. 39 A O ATOM 5117 N TYR 662 64. 602 69. 963 36. 984 1. 00 13. 28 A N ATOM 5119 CB TYR 662 62. 305 69. 143 37. 308 1. 00 13. 28 A N ATOM 5119 CB TYR 662 61. 395 68. 026 36. 862 1. 00 14. 50 A C ATOM 5119 CB TYR 662 61. 395 68. 026 36. 862 1. 00 14. 50 A C ATOM 5119 CB TYR 662 61. 395 68. 026 36. 862 1. 00 14. 50 A C ATOM 5119 CB TYR 662 61. 395 68. 026 36. 862 1. 00 14. 50 A C ATOM 5119 CB TYR 662 61. 395 68. 026 36. 862 1. 00 14. 50 A C ATOM 5119 CB TYR 662 61. 395 68. 026 36. 862 1. 00 14. 50 A C ATOM 5120 CG TYR 662 61. 395 68. 026 36. 862 1. 00 14. 50 A C ATOM 5120 CG TYR 662 61. 395 68. 026 36. 862 1. 00 14. 50 A C ATOM 5120 CG TYR 662 61. 395 68. 026 36. 862 1. 00 14. 50 A C ATOM 5120 CG TYR 662 60. 010 68. 199 36. 802 1. 00 15. 74 A C ATOM 5120 CG TYR 662 61. 395 68. 026 36. 802 1. 00 15. 74 A C ATOM 5120 CG TYR 662 60. 010 68. 199 36. 802 1. 00 15. 74 A C
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ATOM 5104 0 GLU 660 67.001 72.922 36.659 1.00 16.67 A 0 ATOM 5105 N TYR 661 66.539 71.383 38.233 1.00 14.54 A N ATOM 5106 CA TYR 661 67.003 70.269 37.399 1.00 14.57 A C ATOM 5107 CB TYR 661 67.642 69.154 38.230 1.00 13.59 A C ATOM 5108 CG TYR 661 68.878 69.504 39.035 1.00 15.73 A C ATOM 5109 CD1 TYR 661 69.743 70.531 38.655 1.00 13.37 A C ATOM 5110 CE1 TYR 661 70.889 70.805 39.390 1.00 12.74 A C ATOM 5111 CD2 TYR 661 69.199 68.765 40.166 1.00 16.63 A C ATOM 5112 CE2 TYR 661 70.338 69.027 40.898 1.00 16.03 A C ATOM 5113 CZ TYR 661 71.183 70.041 40.515 1.00 13.47 A C ATOM 5114 OH TYR 661 72.322 70.252 41.267 1.00 8.43 A 0 ATOM 5115 C TYR 661 65.842 69.637 36.608 1.00 15.74 A C ATOM 5116 0 TYR 661 66.077 68.854 35.675 1.00 13.97 A 0 ATOM 5117 N TYR 662 64.602 69.963 36.984 1.00 13.28 A N ATOM 5118 CA TYR 662 63.445 69.390 36.308 1.00 13.00 A C ATOM 5119 CB TYR 662 62.305 69.143 37.308 1.00 14.01 A C ATOM 5120 CG TYR 662 61.395 68.026 36.862 1.00 14.50 A C ATOM 5121 CD1 TYR 662 60.010 68.199 36.802 1.00 15.74 A C
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ATOM 5110 CE1 TYR 661 70.889 70.805 39.390 1.00 12.74 A C ATOM 5111 CD2 TYR 661 69.199 68.765 40.166 1.00 16.63 A C ATOM 5112 CE2 TYR 661 70.338 69.027 40.898 1.00 16.03 A C ATOM 5113 CZ TYR 661 71.183 70.041 40.515 1.00 13.47 A C ATOM 5114 OH TYR 661 72.322 70.252 41.267 1.00 8.43 A O ATOM 5115 C TYR 661 65.842 69.637 36.608 1.00 15.74 A C ATOM 5116 O TYR 661 66.077 68.854 35.675 1.00 13.97 A O ATOM 5117 N TYR 662 64.602 69.963 36.984 1.00 13.28 A N ATOM 5118 CA TYR 662 63.445 69.390 36.308 1.00 13.00 A C ATOM 5119 CB TYR 662 62.305 69.143 37.308 1.00 14.01 A C ATOM 5120 CG TYR 662 61.395 68.026 36.862 1.00 14.50 A C ATOM 5121 CD1 TYR 662 60.010 68.199 36.802 1.00 15.74 A C
ATOM 5111 CD2 TYR 661 69.199 68.765 40.166 1.00 16.63 A C ATOM 5112 CE2 TYR 661 70.338 69.027 40.898 1.00 16.03 A C ATOM 5113 CZ TYR 661 71.183 70.041 40.515 1.00 13.47 A C ATOM 5114 OH TYR 661 72.322 70.252 41.267 1.00 8.43 A O ATOM 5115 C TYR 661 65.842 69.637 36.608 1.00 15.74 A C ATOM 5116 O TYR 661 66.077 68.854 35.675 1.00 13.97 A O ATOM 5117 N TYR 662 64.602 69.963 36.984 1.00 13.28 A N ATOM 5118 CA TYR 662 63.445 69.390 36.308 1.00 13.00 A C ATOM 5119 CB TYR 662 62.305 69.143 37.308 1.00 14.01 A C ATOM 5120 CG TYR 662 61.395 68.026 36.862 1.00 14.50 A C ATOM 5121 CD1 TYR 662 60.010 68.199 36.802 1.00 15.74 A C
ATOM 5112 CE2 TYR 661 70.338 69.027 40.898 1.00 16.03 A C ATOM 5113 CZ TYR 661 71.183 70.041 40.515 1.00 13.47 A C ATOM 5114 OH TYR 661 72.322 70.252 41.267 1.00 8.43 A O ATOM 5115 C TYR 661 65.842 69.637 36.608 1.00 15.74 A C ATOM 5116 O TYR 661 66.077 68.854 35.675 1.00 13.97 A O ATOM 5117 N TYR 662 64.602 69.963 36.984 1.00 13.28 A N ATOM 5118 CA TYR 662 63.445 69.390 36.308 1.00 13.00 A C ATOM 5119 CB TYR 662 62.305 69.143 37.308 1.00 14.01 A C ATOM 5120 CG TYR 662 61.395 68.026 36.862 1.00 14.50 A C ATOM 5121 CD1 TYR 662 60.010 68.199 36.802 1.00 15.74 A C
ATOM 5113 CZ TYR 661 71.183 70.041 40.515 1.00 13.47 A C ATOM 5114 OH TYR 661 72.322 70.252 41.267 1.00 8.43 A O ATOM 5115 C TYR 661 65.842 69.637 36.608 1.00 15.74 A C ATOM 5116 O TYR 661 66.077 68.854 35.675 1.00 13.97 A O ATOM 5117 N TYR 662 64.602 69.963 36.984 1.00 13.28 A N ATOM 5118 CA TYR 662 63.445 69.390 36.308 1.00 13.00 A C ATOM 5119 CB TYR 662 62.305 69.143 37.308 1.00 13.00 A C ATOM 5120 CG TYR 662 61.395 68.026 36.862 1.00 14.50 A C ATOM 5121 CD1 TYR 662 60.010 68.199 36.802 1.00 15.74 A C
ATOM 5114 OH TYR 661 72.322 70.252 41.267 1.00 8.43 A 0 ATOM 5115 C TYR 661 65.842 69.637 36.608 1.00 15.74 A C ATOM 5116 O TYR 661 66.077 68.854 35.675 1.00 13.97 A 0 ATOM 5117 N TYR 662 64.602 69.963 36.984 1.00 13.28 A N ATOM 5118 CA TYR 662 63.445 69.390 36.308 1.00 13.00 A C ATOM 5119 CB TYR 662 62.305 69.143 37.308 1.00 14.01 A C ATOM 5120 CG TYR 662 61.395 68.026 36.862 1.00 14.50 A C ATOM 5121 CD1 TYR 662 60.010 68.199 36.802 1.00 15.74 A C
ATOM 5115 C TYR 661 65.842 69.637 36.608 1.00 15.74 A C ATOM 5116 0 TYR 661 66.077 68.854 35.675 1.00 13.97 A 0 ATOM 5117 N TYR 662 64.602 69.963 36.984 1.00 13.28 A N ATOM 5118 CA TYR 662 63.445 69.390 36.308 1.00 13.00 A C ATOM 5119 CB TYR 662 62.305 69.143 37.308 1.00 14.01 A C ATOM 5120 CG TYR 662 61.395 68.026 36.862 1.00 14.50 A C ATOM 5121 CD1 TYR 662 60.010 68.199 36.802 1.00 15.74 A C
ATOM 5116 0 TYR 661 66.077 68.854 35.675 1.00 13.97 A 0 ATOM 5117 N TYR 662 64.602 69.963 36.984 1.00 13.28 A N ATOM 5118 CA TYR 662 63.445 69.390 36.308 1.00 13.00 A C ATOM 5119 CB TYR 662 62.305 69.143 37.308 1.00 14.01 A C ATOM 5120 CG TYR 662 61.395 68.026 36.862 1.00 14.50 A C ATOM 5121 CD1 TYR 662 60.010 68.199 36.802 1.00 15.74 A C
ATOM 5118 CA TYR 662 63.445 69.390 36.308 1.00 13.00 A C ATOM 5119 CB TYR 662 62.305 69.143 37.308 1.00 14.01 A C ATOM 5120 CG TYR 662 61.395 68.026 36.862 1.00 14.50 A C ATOM 5121 CD1 TYR 662 60.010 68.199 36.802 1.00 15.74 A C
ATOM 5119 CB TYR 662 62. 305 69. 143 37. 308 1. 00 14. 01 A C ATOM 5120 CG TYR 662 61. 395 68. 026 36. 862 1. 00 14. 50 A C ATOM 5121 CD1 TYR 662 60. 010 68. 199 36. 802 1. 00 15. 74 A C
ATOM 5120 CG TYR 662 61.395 68.026 36.862 1.00 14.50 A C ATOM 5121 CD1 TYR 662 60.010 68.199 36.802 1.00 15.74 A C
ATOM 5121 CD1 TYR 662 60.010 68.199 36.802 1.00 15.74 A C
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The state of the s
ATOM 5123 CD2 TYR 662 61.930 66.825 36.400 1.00 14.83 A C
ATOM 5124 CE2 TYR 662 61.122 65.830 35.873 1.00 15.13 A C ATOM 5125 CZ TYR 662 59.756 66.024 35.804 1.00 15.11 A C
ATOM FIRE OIL TWO COD SO COD OF COD
ATOM 5126 OH TYR 662 58. 983 65. 060 35. 214 1. 00 17. 05 A O ATOM 5127 C TYR 662 62. 964 70. 251 35. 135 1. 00 12. 46 A C
ATOM 5128 0 TYR 662 63.320 71.423 35.030 1.00 12.22 A 0
ATOM 5129 N ASP 663 62.147 69.673 34.260 1.00 12.09 A N
ATOM 5130 CA ASP 663 61.686 70.394 33.076 1.00 13.20 A C
ATOM 5131 CB ASP 663 60.998 69.427 32.099 1.00 11.88 A C ATOM 5132 CG ASP 663 59.668 68.925 32.606 1.00 13.51 A C
ATOM 5199 OD1 ACD CC9 50 450 00 000 1100 11
ATOM F194 OD9 AGD CC9 F0 CO0 G0 GF0 CO CO
ATOM 5135 C ASP 663 60.807 71.625 33.300 1.00 13.03 A C
ATOM 5136 0 ASP 663 60.036 71.713 34.260 1.00 12.71 A 0
ATOM 5137 N SER 664 60.945 72.576 32.383 1.00 12.83 A N
ATOM 5138 CA SER 664 60.210 73.829 32.425 1.00 13.80 A C ATOM 5139 CB SER 664 60.433 74.600 31.120 1.00 14.92 A C
ATOM ELAO OC COD COL
ATOM 5141 C CPD CC4 TO THE TO COS TO THE THE TO THE
ATOM 5142 0 SER 664 58.234 73.974 33.762 1.00 15.82 A 0
ATOM 5143 N VAL 665 57.987 73.247 31.658 1.00 13.43 A N
ATOM 5144 CA VAL 665 56.540 73.101 31.733 1.00 14.34 A C

					FIC	G. 4-	106			(Continued)
					1, 1 (J. 4	100			
ATOM	5145	CB	VAL	665	56.027	72.182	30.602	1.00 14.98	Α	С
ATOM	5146	CG1		665	54.496	72. 131	30.615	1.00 15.10	Ä	č
ATOM	5147		VAL	665	56. 537	72.690	29. 263	1.00 13.19	A	č
ATOM	5148	C	VAL	665	55. 972	72.620	33. 070	1.00 14.50	A	č
ATOM	5149	ŏ	VAL	665	55. 153	73. 302	33.677	1.00 14.33	A	Ŏ
ATOM	5150	Ň	TYR	666	56. 392	71.452	33. 534	1.00 15.45	A	Ň
ATOM	5151	CA	TYR	666	55. 876	70. 948	34. 801	1.00 17.06	A	Č
ATOM	5152	CB	TYR	666	56. 323	69. 501	35. 038	1.00 15.58	A	č
ATOM	5153	CG	TYR	666	55. 839	68. 903	. 36. 349	1.00 13.36	Ä	C
ATOM	5154		TYR	666	54. 692	68. 119	36. 395	1.00 13.34	A	C
ATOM	5155		TYR	666	54. 276	67. 517	37. 577	1.00 14.70	A	C
ATOM	5156		TYR	666	56. 560	69. 080	37. 534	1.00 13.28		C
ATOM	5157		TYR	666	56. 154	68. 482	38. 727	1.00 13.77	A	C
ATOM	5158	CZ	TYR	666	55. 012	67. 700	38. 737	1.00 12.27	A	C
ATOM	5159	OH	TYR	666	54. 609	67. 072	39. 896	1.00 13.32	A	C
ATOM	5160	C	TYR	666	56. 297	71. 796	35. 998	1.00 18.37	A	0 C
ATOM	5161	Õ	TYR	666	55. 451	72. 200	36. 795		A	
ATOM	5162	N	THR	667	57. 592	72. 266	36. 125	1.00 19.29	A	0 N
ATOM	5163	CA	THR	667	58. 092	72. 833	37. 265	1.00 17.90	A	N
ATOM	5164	CB	THR	667	59. 621	72. 953	37. 251	1.00 19.74	. A	C
ATOM	5165	0G1		667	60. 206	71.675		1.00 18.84	A	C
ATOM	5166		THR	667			36.968 38.604	1.00 20.18 1.00 17.74	A	0
ATOM	5167	C	THR	667	60. 108 57. 537	73. 441 74. 246			A	C
ATOM	5168	0	THR	667	56.916	74. 635	37. 339 38. 333	1.00 21.44	A	C
ATOM	5169	N	GLU	668	57. 7.78			1.00 21.51	A	0
ATOM	5170	CA	GLU	668	57. 330	75.011	36. 280	1.00 21.85	A	N
ATOM	5171	CB	GLU	668	57. 746	76. 389 76. 976	36. 200	1.00 21.18 1.00 20.69	A	C
ATOM	5172	CG	GLU	668	59. 251	77. 096	34. 859 34. 703		A	C
ATOM	5173	CD	GLU		59. 657	77. 559	33. 322	1.00 20.20	A	C
ATOM	5173		GLU	668 668	09.001 E0 709	78. 068		1.00 19.55	A	C
ATOM	5175		GLU	668	58. 783		32. 588	1.00 19.49	A	0
ATOM	5176		GLU	668	60.851	77. 422	32.977	1.00 18.34	A	0
ATOM		C	GLU		55.828	76.517	36. 394	1.00 21.50	A	C
ATOM	5177 5178	0 N	ARG	668	55.339	77. 559	36.814	1.00 22.31	A	0
ATOM	5179	N CA	ARG	669	55.098	75.449	36. 101	1.00 21.90	A	N
ATOM	5180	CB	ARG	669	53.648	75. 458	36. 249	1.00 21.18	A	C
				669	53.060	74. 121	35. 786	1.00 22.06	A	C
ATOM	5181	CC	ARG	669	51.546	74. 026	35. 922	1.00 21.37	A	C
ATOM	5182	CD	ARG	669	51.085	72. 625	35. 653	1.00 20.85	A	Ç
ATOM	5183	NE C7	ARG	669	51.467	72. 187	34. 319	1.00 21.84	A	N
ATOM	5184	CZ	ARG	669	51.667	70.918	33. 981	1.00 21.10	A	Ç
ATOM	5185		ARG	669	51.522	69. 962	34. 888	1.00 19.62	A	N
ATOM	5186		ARG	669	52.018	70.610	32. 741	1.00 20.23	A	N
ATOM	5187	C	ARG	669	53. 246	75. 706	37. 695	1.00 21.23	A	C
ATOM	5188	0 M	ARG	669	52. 209	76. 306	37. 957	1.00 20.45	A	0
ATOM	5189	N	TYR	670	54.067	75. 239	38. 631	1.00 21.65	Ą	N
ATOM	5190	CA	TYR	670	53. 771	75. 409	40.047	1.00 22.27	A	C
ATOM	5191	CB	TYR	670	53. 752	74.048	40.764	1.00 21.10	Ą	C
ATOM	5192	CCD1	TYR	670	53. 113	72. 930	39. 972	1.00 20.47	Ą	C
ATOM	5193	CD1	ПК	670	53. 896	71.995	39. 310	1.00 20.74	Α	С

				FIG	. 4 -	107			(Continued)
ATOM ATOM ATOM	5194 5195 5196	CE1 T CD2 T CE2 T	TYR 670 TYR 670	53. 321 51. 726 51. 139	70. 985 72. 831 71. 831	38. 537 39. 850 39. 079	1.00 22.18 1.00 19.78 1.00 19.87	A A A	C C C
ATOM ATOM ATOM	5197 5198 5199	ОН Т	FYR 670 FYR 670 FYR 670	51.388	70. 911 69. 931 76. 317	38. 422 37. 623 40. 757	1.00 22.17 1.00 23.11 1.00 23.32	A A A	C 0 C
ATOM ATOM	5200 5201	0 I N M	TYR 670 ÆT 671	54. 442 55. 983	76. 937 76. 404	41. 763 40. 228	1.00 24.86 1.00 24.66	A A	O N
ATOM ATOM ATOM	5202 5203 5204	CB M	ÆT 671 ÆT 671 ÆT 671	58. 327	77. 207 76. 400 75. 215	40. 851 40. 905 41. 852	1. 00 23. 96 1. 00 24. 00 1. 00 23. 55	A A A	C C C
ATOM ATOM ATOM	5205 5206 5207	CE M	ÆT 671 ÆT 671 ÆT 671	58. 383 60. 159	75. 732 75. 998 78. 547	43. 565 43. 721 40. 203	1. 00 24. 97 1. 00 21. 94 1. 00 24. 00	A A	S C C
ATOM ATOM	5208 5209	O M N G	ÆT 671 SLY 672	58. 101 56. 741	79. 331 78. 822	40. 756 39. 045	1.00 25.98 1.00 22.07	A A A	O N
ATOM ATOM ATOM	5210 5211 5212	C G	ELY 672 ELY 672 ELY 672	58.472	80. 076 80. 028 78. 947	38. 379 37. 857 37. 641	1. 00 22. 40 1. 00 22. 69 1. 00 23. 27	A A A	C C O
ATOM ATOM ATOM	5213 5214 5215	CA L	.EU 673 .EU 673 .EU 673	60. 477	81. 180 81. 209 82. 356	37. 667 37. 151 36. 164	1.00 22.65 1.00 20.90 1.00 19.50	A A A	N C C
ATOM ATOM	5216 5217	CG L CD1 L	.EU 673 .EU 673	59. 639 59. 779	82. 282 83. 513	35. 010 34. 147	1.00 19.96 1.00 20.87	A A	C C
ATOM ATOM ATOM	5218 5219 5220	0 L	EU 673 EU 673	61.528 61.313	81. 027 81. 344 82. 028	34. 203 38. 248 39. 239	1.00 21.63 1.00 21.08 1.00 21.87	A A A	C C O
ATOM ATOM ATOM	5221 5222 5223	CD P	RO 674 RO 674 RO 674	63.050	80. 700 79. 803 80. 747	38. 072 36. 968 39. 050	1.00 21.90 1.00 21.16 1.00 23.23	A A A	N C C
ATOM ATOM ATOM	5224 5225 5226	CB P	RO 674 RO 674	64. 618 63. 803	79. 510 78. 755	38. 709 37. 695	1.00 21.90 1.00 22.34	A A	C C
ATOM ATOM	5227 5228	O P N T	RO 674 RO 674 HR 675	65. 841 8 63. 966 8	82. 023 81. 977 83. 158	38. 943 39. 028 38. 743	1.00 24.90 1.00 26.10 1.00 25.88	A A A	C O N
ATOM ATOM ATOM	5229 5230 5231	CA TO CB TO CG1 TO	HR 675	64. 208	84. 411 85. 237 85. 524	38. 640 37. 447 37. 599	1.00 27.60 1.00 27.12 1.00 29.30	A A A	C C 0
ATOM ATOM ATOM	5232 5233 5234	CG2 T		64. 431 8 64. 496 8	84. 471 85. 211 84. 982	36. 156 39. 918 40. 660	1.00 25.59 1.00 28.74	A A	C C
ATOM ATOM	5235 5236	N P	RO 676 RO 676	65.404 8 66.625 8	36. 156 36. 508	40. 200 39. 457	1. 00 29. 47 1. 00 29. 41 1. 00 28. 96	A A A	O N C
ATOM ATOM ATOM	5237 5238 5239	CB P	RO 676 RO 676 RO 676	66.465	36.969 37.929 37.142	41.411 41.299 40.533	1. 00 29. 70 1. 00 28. 87 1. 00 28. 27	A A A	C C C
ATOM ATOM ATOM	5240 5241 5242	0 P	RO 676 RO 676 LU 677	63.359	37. 707 37. 829 38. 190	41.484 42.558 40.343	1.00 30.03 1.00 29.93 1.00 30.62	A A A	C O N

						•					(Cont	tinued)
	**				FIC	. 4 -	108					
ATOM	5243	CA G	LU 6'	77 6	2. 203	88. 923	40.348		30.92	A	C	
ATOM	5244	CB G			2. 192	90.013	39. 264		32.38	Ą	C	
ATOM	5245				2. 103	89. 536	37. 821		34. 78	A	C	
ATOM	5246				3. 380	88. 877	37. 331		37.04	A	C	
ATOM	5247	0E1 G			4. 480	89. 356	37.697		35.11	A	0	
ATOM	5248	OE2 G			3. 276	87. 891	36.566		37. 80	A	0 C	
ATOM	5249				50. 952	88.065	40. 231		30.10	A	0	
ATOM	5250				9. 893	88. 564	39.849		31.67 28.40	A A	N	
ATOM	5251				51.067 59.906	86. 777 85. 897	40. 546 40. 523		26. 09	A	Č	
ATOM	5252				59. 833	85. 048	39. 253		25.88	A	Č	
ATOM	5253				58. 472	84. 359	39. 097		28. 22	A	Č	
ATOM	5254 5255	OD1 A			57. 885	83. 980	40. 128		28.64	A	ŏ	
ATOM ATOM	5256	0D2 A			57. 980	84. 189	37. 956		28. 80	Ä	Õ	
ATOM	5257				59. 920	84. 982	41.737		25.86	A	Č	
ATOM	5258				59. 481	85. 382	42.810		28.55	. A	. 0	
ATOM	5259				60. 442	83. 768	41.591		23.97	Α	N	
ATOM	5260				50. 443	82.835	42.708		21.47	Α	С	
ATOM	5261				59.326	81.818	42.496	1.00	19.41	Α	С	
ATOM	5262				58. 894	81.146	43.778	1.00	19.58	Α	С	
ATOM	5263	0D1 A			58. 491	79.981			20.44	Α	0	
ATOM	5264	ND2 A		79	58.957	81.879	44.882		18.70	Α	N	
ATOM	5265	C A			61.760	82.099	42.957		21.79	A	C	
ATOM	5266				61.770	81.055	43.601		21.89	A	0	
ATOM	5267				62.873	82.636	42.472		24.38	A	И.	
ATOM	5268				64. 164	81.967	42.665		26. 33	A	C	
ATOM	5269				65.316	82.842	42. 157		26. 74	A	C	
ATOM	5270				66. 726	82. 275	42.385		28. 22	A	C	
ATOM	5271	CD1 I			66.844	80.903	41.747		30.03 29.33	A	C	
ATOM	5272	CD2 I			67.772	83. 211 81. 556	41.801		27.18	A A	Č	
ATOM	5273				64. 449 64. 977	80. 471	44. 103		28.31	A	0	
ATOM	5274				64. 111	82.411	45.072		27. 79	A	N	
ATOM ATOM	5275 5276				64. 360	82. 091	46. 475		28. 03	A	Č	
ATOM	5277				63.836	83. 196	47. 394		30.36	Ä	č	
ATOM	5278				64. 774	84. 386	47. 473		34. 23	A	č	
ATOM	5279	0D1 A		81	65. 908	84. 289			35. 59	A		
ATOM	5280	OD2 /			64. 380	85. 417	48.067		36.71	A	Ō	
ATOM	5281				63.773	80.753	46.920		27.55	Α	Ċ	
ATOM	5282				64. 428	80.005	47.647	1.00	28.05	Α	0	
ATOM	5283				62.551	80.438	46.502	1.00	25.37	Α	N	
ATOM	5284				61.981	79. 164	46.913		25.07	Α	С	
ATOM	5285			882	60.456	79.161	46.801		25. 14	Α	С	
ATOM	5286	CG I	HIS 6		59.832	77.914	47.349		27. 18	A	C	
ATOM	5287	CD2 I			59. 091	76. 948	46.754		27. 87	A	C	
ATOM	5288	ND1 I			60.021	77. 503	48.650		26. 29	A	N	
ATOM	5289	CE1 I			59.428	76. 336	48.832		26.61	A	Ç	
ATOM	5290	NE2			58.857	75.977	47.697		25.03	A	N	
MOTA	5291	C 1	HIS (882	62.559	77. 983	46.130	1.00	24. 30	A	С	

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	t				TO T 4	~ 4 -	1 0 0			(Continued)
					r I (G. 4-	109			
ATOM	5292	0	HIS	682	62.463		46.572	1.00 23.47	Α	0
ATOM	5293	N	TYR	683	63.144		44.966	1.00 23.49	A	N
ATOM	5294	CA	TYR	683	63. 768		44. 157	1.00 22.64	A	C
ATOM	5295	CB	TYR	683	64. 249		42.812	1.00 20.68	A	C
ATOM ATOM	5296 5297	CG CD1	TYR	683	63. 291	77. 594	41.655	1.00 19.28 1.00 16.29	A	C
ATOM	5298	CE1		683 683	63. 325 62. 464	76. 461 76. 317	40.857 39.783	1.00 16.29	A A	C C
ATOM	5299	CD2		683	62. 361	78. 589	41.347	1.00 10.63	A	C
ATOM	5300	CE2		683	61.495	78. 453	40. 276	1.00 20.47	A	Č
ATOM	5301	CZ	TYR	683	61.554		39.500	1.00 19.09	A	č
ATOM	5302	OH	TYR	683	60.695	77.176	38. 441	1.00 21.54	A	Ŏ
ATOM	5303	С	TYR	683	64.989	76. 727	44.924	1.00 22.32	Ā	Č
ATOM	5304	0	TYR	683	65.189	75. 533	45.125	1.00 22.65	A	0
ATOM	5305	N	ARG	684	65. 799	77. 685	45. 355	1.00 22.44	Α	N
ATOM	5306		ARG	684	67. 025	77. 392	46.076	1.00 22.97	Α	C
ATOM	5307		ARG	684	67. 928	78. 624	46.071	1.00 22.89	A	C
ATOM	5308		ARG	684	68. 349	79.064	44.672	1.00 24.57	A	C
ATOM	5309		ARG	684	69. 238	78. 020	44.004	1.00 23.11	A	C
ATOM ATOM	5310 5311		ARG ARG	684	69. 328	78. 223	42.562	1.00 25.47	A	N C
ATOM	5312	NH1		684 684	69. 844 70. 337	79. 299 80. 294	41. 974 42. 703	1.00 27.89 1.00 29.09	A	C
ATOM	5313	NH2		684	69. 846	79. 388	40. 648	1.00 23.03	A A	N N
ATOM	5314		ARG	684	66. 807	76. 922	47. 501	1.00 21.04	A	Č
ATOM	5315		ARG	684	67. 711	76. 368	48. 111	1.00 24.16	A	ŏ
ATOM	5316		ASN	685	65.608	77. 121	48. 030	1.00 24.64	A	Ň
ATOM	5317	CA	ASN	685	65. 331	76.715	49.399	1.00 24.41	A	Ċ
ATOM	5318		ASN	685	64. 599	77.831	50.134	1.00 28.42	. A	C
ATOM	5319		ASN	685	64. 455	77. 547	51.610	1.00 34.24	Α	C
ATOM	5320	OD1		685	65. 410	77. 117	52. 266	1.00 38.25	, A	0
ATOM	5321	ND2		685	63. 264	77. 791	52. 150	1.00 37.49	A	N
ATOM	5322		ASN	685	64. 545	75. 419	49.537	1.00 23.72	A	C
ATOM ATOM	5323 5324		ASN SER	685	64. 356	74. 929	50.649	1.00 23.86	A	0
ATOM	5325		SER	686 686	64. 101 63. 336	74. 852 73. 613	48. 417 48. 457	1.00 21.55 1.00 19.71	A	N
ATOM	5326		SER	686	61.976	73.811	47. 774	1.00 19.71	A A	C C
ATOM	5327		SER	686				1.00 15.20	A	Ö
ATOM	5328		SER	686	64.060	72. 421	47. 823	1.00 20.13	A	Č
ATOM	5329		SER	686	63. 447	71.611	47. 128	1.00 21.27	Ä	ŏ
ATOM	5330		THR	687	65. 362	72.307	48.060	1.00 19.02	Ä	Ň
ATOM	5331		THR	687	66.122	71.189	47.509	1.00 17.15	Ā	C
ATOM	5332		THR	687	67. 441	71.665	46.906	1.00 16.10	A	Č
ATOM	5333	0G1		687	68. 362	71.959	47.960	1.00 17.42	Α	0
ATOM	5334	CG2		687	67. 214	72. 920	46.058	1.00 14.71	A	C
ATOM	5335		THR	687	66. 433	70. 153	48. 585	1.00 15.79	A	C
ATOM	5336		THR	687	66. 496	70.466	49. 763	1.00 15.82	A	0
ATOM ATOM	5337 5338		VAL VAL	688 688	66. 627	68. 908	48. 182	1.00 18.43	A	N
ATOM	5339		VAL VAL	688	66. 935 66. 840	67.854	49.147	1.00 17.92	A	C
ATOM	5340	CG1		688	67. 092	66. 453 65. 352	48. 480 49. 503	1.00 17.13 1.00 15.01	. A . A	C C
111 014	VO 10	JU1		500	01.032	UU. JUL	40.009	1.00 10.01	· п	U

					FIC	G. 4-	110			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5341 5342 5343 5344 5345 5346 5346 5351 5353 5354 5355 5356 5356 5360 5362 5363 5364 5365	O N CA CB CC O N CA CB CC O N CA CB CC CD N CA CB CC CD N CA CB CC CD N CC CC CD CC	VAL VAL MET MET MET MET MET MET MET MET SER SER SER ARG ARG ARG ARG ARG	688 688 689 689 689 689 689 690 690 690 691 691 691 691	65. 459 68. 341 68. 559 69. 280 70. 672 71. 475 71. 829 70. 465 70. 338 70. 897 71. 721 70. 179 70. 358 69. 621 68. 234 69. 898 69. 930 69. 480 69. 041 67. 591 66. 623 65. 201 64. 236 62. 963	68. 210 67. 740 69. 210 69. 539 69. 220 70. 653 71. 544 72. 866 72. 702 70. 933 71. 606 69. 672 69. 012 68. 546 69. 652 69. 152 70. 240 70. 134	47. 845 49. 720 50. 923 48. 851 49. 246 48. 065 46. 984 45. 909 44. 871 50. 569 51. 712 51. 501 51. 711 53. 038 54. 063 53. 023 54. 249 54. 113 53. 770 53. 813 53. 694 54. 061	1. 00 18. 49 1. 00 17. 50 1. 00 15. 69 1. 00 16. 92 1. 00 17. 40 1. 00 13. 91 1. 00 10. 55 1. 00 11. 73 1. 00 9. 36 1. 00 17. 90 1. 00 16. 90 1. 00 18. 32 1. 00 21. 65 1. 00 20. 29 1. 00 24. 78 1. 00 22. 31 1. 00 23. 43 1. 00 21. 70 1. 00 23. 07 1. 00 22. 90 1. 00 22. 81 1. 00 22. 97 1. 00 24. 03 1. 00 25. 20	A A A A A A A A A A A A A A A A A A A	C C C O N C C C C C O N C C C C C N C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5362 5363 5364 5365 5366 5367 5368 5369 5370 5371 5372 5373 5374 5375	CD NE CZ NH1 NH2 C O N CA CB CC CB CC CD OE1	ARG ARG ARG ARG	691 691	65. 201 64. 236	69. 152 70. 240 70. 134 68. 989 71. 172 67. 811 67. 031 67. 675 66. 561 66. 826 66. 210 65. 068 67. 181 66. 944 68. 266 68. 606 67. 627 66. 948 67. 554 66. 215 65. 505 66. 387	53. 813 53. 694	1.00 24.03	Α	N
ATOM ATOM ATOM ATOM ATOM	5385 5386 5387 5388 5389	CB CG OD1	ASN ASN ASN ASN ASN	694 694 694 694 694	68. 274 68. 191 67. 291 69. 127 69. 412	66. 473 67. 796 68. 607 68. 015	58. 619 59. 370 59. 132 60. 287 58. 567	1.00 26.79 1.00 28.23 1.00 29.60 1.00 27.09 1.00 22.78	A A A A	C C O N C

				FIG.	4 -	111			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5426 5427	O AS N PH CA PH CB PH CCD PH CCD PH CCD PH CCD PH CCD LY CC U CE U CO CC U CE U CO CC U CO C U CO C U CO C U CO C U C U C U C U C U C U C U C U C U C U	世 695 695 695 695 695 695 695 695 695 696 696	68. 736 6 70. 008 6 69. 876 6 70. 297 6 69. 262 6 68. 980 6 68. 582 6 68. 033 6 67. 636 6 67. 360 6 70. 704 6 70. 734 6 71. 388 6 72. 189 6 73. 119 6 74. 230 6 75. 160 6 76. 354 6 77. 248 6 71. 256 6 71. 673 5 69. 986 69. 013 6 68. 072 6 68. 072 6 68. 766 6 67. 790 6 68. 086 6 67. 790 6 68. 086 6 67. 294 5 68. 176 5 67. 294 5 68. 439 5 67. 659 5 66. 510 5 65. 674 5 67. 077 68. 469 5 69. 614 5 67. 850 5	3. 555 3. 764 2. 351 2. 085 3. 465 3. 480 4. 160 9. 165 3. 478 3. 165 4. 253 4. 211 2. 385 3. 793 4. 211 2. 865 3. 478 3. 478 9. 790 9. 790 9. 790 9. 233 6. 987 7. 265 5. 868	59. 318 57. 481 57. 135 55. 686 54. 663 54. 394 53. 948 53. 419 52. 976 52. 710 58. 068 57. 932 59. 014 59. 980 60. 744 59. 891 60. 672 59. 816 60. 534 60. 949 61. 865 62. 385 62. 792 63. 262 63. 195 63. 753 61. 259 61. 923 60. 011 59. 383 58. 524 59. 355 57. 296 58. 484 58. 135 58. 121	1. 00 22. 09 1. 00 21. 23 1. 00 20. 87 1. 00 18. 97 1. 00 15. 41 1. 00 16. 20 1. 00 13. 85 1. 00 15. 80 1. 00 14. 69 1. 00 14. 36 1. 00 22. 75 1. 00 23. 86 1. 00 24. 30 1. 00 26. 74 1. 00 26. 74 1. 00 26. 44 1. 00 28. 88 1. 00 24. 58 1. 00 24. 58 1. 00 24. 58 1. 00 24. 58 1. 00 24. 58 1. 00 24. 79 1. 00 37. 16 1. 00 36. 42 1. 00 24. 79 1. 00 27. 00 1. 00 37. 16 1. 00 36. 42 1. 00 24. 79 1. 00 27. 00 1. 00 37. 16 1. 00 36. 42 1. 00 18. 56 1. 00 19. 77 1. 00 19. 77 1. 00 18. 56 1. 00 18. 57 1. 00 18. 57 1. 00 18. 57 1. 00 18. 57 1. 00 18. 57 1. 00 18. 52	A A A A A A A A A A A A A A A A A A A	O N C C C C C C C C O N C C C C C O N C O N C C C C
ATOM ATOM ATOM ATOM ATOM ATOM	5427 5428 5429 5430 5431 5432	CA GI CB GI CG GI CD GI OE1 GI	LU 699 LU 699 LU 699 LU 699 LU 699	68. 456 5 68. 007 5 67. 600 5 68. 384 5 69. 620 5	4. 885 3. 488 3. 411 2. 377 2. 305	57. 236 57. 636 59. 097 59. 891 59. 712	1. 00 18. 24 1. 00 19. 38 1. 00 26. 18 1. 00 29. 91 1. 00 31. 51	A A A A	C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5432 5433 5434 5435 5436 5437 5438	OE1 GI OE2 GI C GI O GI N TY CA TY	LU 699 LU 699 LU 699 /R 700 /R 700	67. 765 5 67. 857 5 66. 638 5 68. 714 5 68. 275 5	2. 305 1. 651 5. 286 5. 397 5. 516 5. 968 7. 383	59. 712 60. 703 55. 891 55. 765 54. 899 53. 584 53. 365	1.00 31.51 1.00 30.28 1.00 17.20 1.00 16.35 1.00 15.53 1.00 12.51 1.00 12.28	A A A A A	0 0 C 0 N C C

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				FIC	G. 4-	112			(Continued)
ATOM	5439	CG TY	/R 700	68. 374	58. 105	52.114	1.00 13.03	A	С
ATOM	5440	CD1 TY		67.027	58.171	51.746	1.00 12.78	Α	C
ATOM	5441	CE1 TY	r 700	66.611	58. 961	50.666	1.00 7.94	Ą	Ċ
ATOM	5442	CD2 TY		69. 301	58.840	51.359	1.00 12.91	A	C
ATOM	5443	CE2 TY		68. 895	59.629	50. 282	1.00 10.45	A	C
ATOM	5444	CZ TY		67. 550		49.948	1.00 10.05	A	C
ATOM	5445	OH TY		67. 150		48. 913	1.00 8.37	A	0
ATOM	5446	C TY		68. 743		52.468	1.00 11.71	A	C
ATOM	5447	0 TY		69.881		52.463	1.00 10.84	A	0
ATOM	5448	N LE		67. 836		51.540	1.00 11.32	A	N
ATOM	5449	CA LI		68.142		50. 383	1.00 11.03	A	C C
ATOM	5450	CB LF		67.313		50.378	1.00 8.96 1.00 10.04	A	C
ATOM	5451	CG LE		67.439	51.794 51.873	49. 123 48. 511	1.00 10.04	A A	C
ATOM	5452	CD1 LH		68. 841 67. 089	50.376	49. 490	1.00 7.25	A	C
ATOM	5453 5454	CD2 LE		67.811	54. 799	49. 170	1.00 13.03	A	č
ATOM ATOM	5454 5455	0 LI		66.660		48. 986	1.00 13.35	A	ŏ
ATOM	5456	N LI		68. 840		48. 367	1.00 12.91	Ä	Ň
ATOM	5457	CA LI		68. 724		47.169	1.00 11.74	A	Ċ
ATOM	5458	CB LI		69. 806		47. 196	1.00 11.17	Ä	č
ATOM	5459	CG LI		69. 916		46.044	1.00 12.13	A	Č
ATOM	5460	CD1 LI		68. 569		45.803	1.00 10.71	Ā	Č
ATOM	5461	CD2 LI		71.006		46.368	1.00 10.37	Α	C
ATOM	5462	C LI		68.883		45.942	1.00 13.49	Α	C
ATOM	5463	0 LI		69.854		45.832	1.00 14.04	Α	0
ATOM	5464	N II	LE 703	67. 935		45.016	1.00 13.82	Α	N
ATOM	5465		LE 703	67. 934		43.806	1.00 12.92	A	С
ATOM	5466		LE 703	66. 931		43. 964	1.00 12.98	A	C
ATOM	5467	CG2 II		66. 897		42.706	1.00 15.12	A	C
ATOM	5468	CG1 II		67. 299		45. 196	1.00 13.52	A	C
ATOM	5469	CD1 II		66. 202		45.663	1.00 13.28	A	C
ATOM	5470		LE 703	67. 561		42.582	1.00 14.12	A	C
ATOM	5471		LE 703	66. 635		42.629	1.00 15.85	A	0
ATOM	5472	N H				41.473	1.00 13.28 1.00 11.81	A	N C
ATOM	5473	CA H				40. 265 40. 391	1.00 11.81	A A	C
ATOM	5474 5475	CB H		67. 968		39.667	1.00 11.13		^
ATOM ATOM	5475 5476	CG H CD2 H		67. 446		38. 418	1.00 11.00	A A	C
ATOM	5477	ND1 H		67. 736		40. 244	1.00 10.03	A	N
ATOM	5478	CE1 H		67. 098		39. 385	1.00 9.04	A	Č
ATOM	5479	NE2 H		66. 910		38. 270	1.00 11.23	A	Ň
ATOM	5480		IS 704	68. 464		38. 992	1.00 11.87	Ä	Ċ
ATOM	5481		IS 704	69. 503		38. 980	1.00 11.87	Ä	ŏ
ATOM	5482		LY 705	67. 684		37. 926	1.00 11.49	Ä	Ň
ATOM	5483		LY 705	68. 075		36.663	1.00 11.90	A	Ċ
ATOM	5484		LY 705	69.066		36.036	1.00 12.16	Α	Č
ATOM	5485		LY 705	68.911	56.660	36.153	1.00 13.94	Α	0
ATOM	5486	N T	HR 706	70. 086		35. 372	1.00 13.29	A	N
ATOM	5487	CA T	HR 706	71.101	55. 782	34. 770	1.00 12.51	A	C

				E.C. 4 110	(Continued)
				FIG. 4-113	
ATOM ATOM	5488 5489			72.417 55.001 34.557 1.00 11.94	A C
ATOM	5490				A 0
ATOM	5491				A C A C
ATOM .					A 0
ATOM	5493			an	A N
ATOM	5494		707		A C
ATOM	5495				A Č
ATOM	5496				Ä · Č
MOTA	5497		707	00 151 00 000 00 000 1 00 1	A 0
ATOM	5498		708	67.764 57.600 32.828 1.00 16.33	A N
ATOM	5499		708	66.534 58.314 33.113 1.00 16.71	A C
ATOM	5500		708		A C
ATOM	5501	CG ASP	708		A C
ATOM	5502	OD1 ASP	708		A 0
ATOM	5503	OD2 ASP	708	64. 498 58. 317 36. 038 1. 00 19. 68	A 0
ATOM	5504	C ASP	708	05 101 00 015 00 010 1	A C
ATOM ATOM	5505	O ASP	708		A 0
ATOM	5506 5507	N ASP	709		A N
ATOM	5508	CA ASP CB ASP	709 709	OF 000 40 MAG 40 40 4 1	A C
ATOM	5509	CG ASP	709		A C
ATOM	5510	OD1 ASP	709	00 010 00 100 00 000	A C
ATOM	5511	OD2 ASP	709	00 500 50 501 05 505	A 0
ATOM	5512	C ASP	709	04 000 04 004 04 400 4 05	A 0
ATOM	5513	0 ASP	709	04 040 00 440 00 700	A C A O
ATOM	5514	N ASN	710	00 010 01 100 00 001	A N
ATOM	5515	CA ASN	710	00 501 00 001 00	A C
ATOM	5516	CB ASN	710	01 500 01 100 00 00	A C
ATOM	5517	CG ASN	710	00 000 00 000 00 000	Ä Č
ATOM	5518	OD1 ASN	710	ED 054 04 500 00 00 00 00 00 00 00 00 00 00 00 00	Ă Ŏ
ATOM	5519	ND2 ASN	710	00 004 00 000 00 000	A N
ATOM	5520	C ASN	710	63. 395 63. 010 33. 938 1. 00 13. 10	A C
ATOM	5521	0 ASN	710	63. 691 64. 211 33. 912 1. 00 12. 53	A 0
ATOM	5522	N VAL	711		A N
ATOM	5523	CA VAL	711	64. 221 62. 741 36. 225 1. 00 9. 96	A C
ATOM	5524	CB VAL	711	63. 620 62. 128 37. 512 1. 00 9. 85 A	
ATOM	5525	CG1 VAL	711	64. 415 62. 570 38. 719 1. 00 7. 61 A	
ATOM ATOM	5526 5527	CG2 VAL	711	62. 176 62. 567 37. 675 1. 00 11. 26 A	
ATOM	5527 5528	C VAL O VAL	711	65. 645 62. 237 36. 038 1. 00 10. 48 A	
ATOM	5529	N HIS	711 712	65. 949 61. 068 36. 280 1. 00 10. 00 A	
ATOM	5530	CA HIS	712	66.518 63.126 35.591 1.00 10.94 A 67.899 62.758 35.302 1.00 11.74 A	
ATOM	5531	CB HIS	712		
ATOM	5532	CG HIS	712		
ATOM	5533	CD2 HIS	712	67. 782 64. 529 33. 514 1. 00 11. 58 A 66. 855 63. 955 32. 705 1. 00 12. 39 A	
ATOM	5534	ND1 HIS	712	67. 833 65. 858 33. 154 1. 00 11. 87 A	
ATOM	5535	CE1 HIS	712	66. 966 66. 082 32. 181 1. 00 12. 19 A	
ATOM	5536	NE2 HIS	712	66. 359 64. 944 31. 891 1. 00 11. 62 A	
				11 02 02.001 11.00 11.00	

				FIG. 4-115	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5587 (6588 N 5589 C 5591 C 5595 C 5596 N 5597 C 5602 N 5603 C 5604 C 5605 C 5606 C 5607 C 5608 N 5609 C 5611 N 5612 C 5613 C 5614 C 5615 C 5616 N 5617 C 5618 C 561	N LYS CA LYS CB LYS CB LYS CC LYS CE LYS CC	718 719 719 719 719 719 719 719 719 720 720 720 720 721 721 721 721 721 721 721 721 721 722 722	73. 350 65. 343 45. 026 1. 00 13. 24 A 73. 941 65. 910 45. 949 1. 00 11. 74 A 72. 370 64. 460 45. 237 1. 00 12. 01 A 71. 956 64. 110 46. 594 1. 00 11. 94 A 70. 691 63. 201 46. 616 1. 00 12. 50 A 70. 464 62. 673 48. 021 1. 00 11. 09 A 69. 447 63. 979 46. 174 1. 00 14. 37 A 68. 170 63. 143 46. 154 1. 00 8. 64 A 73. 081 63. 338 47. 282 1. 00 11. 72 A 73. 543 63. 703 48. 367 1. 00 10. 69 A 73. 508 62. 262 46. 632 1. 00 11. 35 A 74. 557 61. 405 47. 155 1. 00 11. 02 A 74. 901 60. 325 46. 135 1. 00 10. 89 A 75. 471 60. 894 44. 970 1. 00 13. 75 A 76. 429 61. 995 48. 537 1. 00 11. 68 A 76. 159 63. 129 46. 594 1. 00 12. 18 A 77. 336 63. 951 46. 800 1. 00 12. 15 A 77. 613 64. 823 45. 571 1. 00 11. 24 A 78. 764 65. 796 45. 756 1. 00 7. 41 A 79. 517 66. 064 44. 451 1. 00 9. 30 A 78. 674 66. 765 43. 392 1. 00 13. 24 A 78. 341 68. 165 43. 739 1. 00 9. 54 A 77. 190 64. 816 48. 038 1. 00 13. 24 A 78. 341 68. 165 43. 739 1. 00 9. 54 A 77. 190 64. 816 48. 038 1. 00 13. 24 A 78. 341 68. 165 43. 739 1. 00 9. 54 A 77. 190 64. 816 48. 038 1. 00 13. 24 A 78. 341 68. 165 43. 739 1. 00 9. 54 A 77. 190 64. 816 48. 038 1. 00 13. 24 A 78. 341 68. 165 43. 739 1. 00 9. 30 A 78. 674 66. 765 43. 392 1. 00 8. 74 A 78. 341 68. 165 43. 739 1. 00 9. 54 A 77. 190 64. 816 48. 038 1. 00 13. 24 A 78. 341 68. 165 43. 739 1. 00 9. 37 A 75. 874 65. 369 50. 702 1. 00 14. 04 A 76. 430 65. 826 51. 694 1. 00 15. 43 A 75. 360 64. 145 50. 665 1. 00 14. 96 A 75. 429 63. 266 51. 826 1. 00 17. 23 A 74. 626 61. 984 51. 570 1. 00 16. 86	CONCCCCCONCCONCCCCNCONCCCONCC
ATOM ATOM ATOM	5619 C 5620 C 5621 C	G LEU Di LEU D2 LEU	723 723 723	73. 116 62. 205 51. 463 1. 00 18. 78 A 72. 428 60. 932 50. 991 1. 00 18. 74 A 72. 576 62. 663 52. 817 1. 00 16. 86 A	C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM		LEU VAL A VAL B VAL G1 VAL G2 VAL	723 724 724 724 724 724 724 724	76. 889 62. 926 52. 134 1. 00 17. 26 A 77. 320 62. 990 53. 280 1. 00 18. 48 A 77. 641 62. 559 51. 103 1. 00 17. 41 A 79. 050 62. 234 51. 257 1. 00 16. 64 A 79. 671 61. 824 49. 902 1. 00 14. 31 A 81. 187 61. 819 49. 987 1. 00 13. 56 A 79. 178 60. 449 49. 519 1. 00 14. 78 A 79. 785 63. 455 51. 803 1. 00 18. 83 A	C O N C C C C C
ATOM ATOM ATOM ATOM ATOM	5630 O 5631 N 5632 CA 5633 CI 5634 CO	VAL ASP A ASP B ASP	724 725 725 725 725 725	80. 665 63. 337 52. 662 1. 00 19. 09 A 79. 411 64. 632 51. 318 1. 00 19. 19 A 80. 051 65. 848 51. 776 1. 00 20. 26 A 79. 627 67. 032 50. 919 1. 00 22. 40 A 80. 259 67. 004 49. 549 1. 00 26. 44 A	O N C C

				FIG. 4-116		(Continued)
АТОИ	5635	OD1 ASP	725	81.149 66.151 49.319 1.00 26.28	Α	0 .
ATOM ATOM	5636	OD2 ASP	725	79. 867 67. 839 48. 704 1. 00 30. 70	A	0
ATOM	5637	C ASP	725	79. 805 66. 171 53. 238 1. 00 19. 86	Α	C
ATOM	5638	0 ASP	725	80. 486 67. 024 53. 792 1. 00 23. 33	Α	0
ATOM	5639	N VAL	726	78. 841 65. 516 53. 873 1. 00 17. 95	Α	N
ATOM	5640	CA VAL	726	78.603 65.790 55.285 1.00 17.97	Α	С
ATOM	5641	CB VAL	726	77. 178 66. 341 55. 567 1. 00 18. 54	Α	C
ATOM	5642	CG1 VAL	726	76.992 67.680 54.875 1.00 16.64	Α	C
ATOM	5643	CG2 VAL	726	76. 121 65. 339 55. 120 1. 00 18. 24	Α	C
ATOM	5644	C VAL	726	78.812 64.549 56.124 1.00 17.82	A	C
ATOM	5645	0 VAL	726	78. 412 64. 504 57. 283 1. 00 19. 86	A	0
ATOM	5646	N GLY	727	79. 439 63. 541 55. 535 1. 00 17. 13	A	N
ATOM	5647	CA GLY	727	79.711 62.317 56.263 1.00 16.84	A	C
ATOM	5648	C GLY	727	78.509 61.489 56.681 1.00 17.94	A	C
ATOM	5649	0 GLY	727	78. 483 60. 961 57. 794 1. 00 19. 74	A	0
ATOM	5650	N VAL	728	77. 517 61. 371 55. 802 1. 00 16. 62	A	N C
ATOM	5651	CA VAL	728	76. 331 60. 571 56. 085 1. 00 17. 26	A	C C
ATOM	5652	CB VAL	728	75. 030 61. 302 55. 643 1. 00 18. 46 73. 838 60. 338 55. 668 1. 00 16. 22	A A	C
ATOM	5653	CG1 VAL	728		A	C
ATOM	5654	CG2 VAL	728	· - · · · · · · · · · · · · · · · · · ·	A	Č
ATOM	5655	C VAL	728	76. 411 59. 230 55. 347 1. 00 18. 03 76. 667 59. 186 54. 143 1. 00 18. 40	A	Ö
ATOM	5656	O VAL	728 729	76. 211 58. 135 56. 069 1. 00 18. 22	A	· N
ATOM	5657	N ASP CA ASP	729	76. 246 56. 822 55. 441 1. 00 19. 90	A	Ċ
ATOM ATOM	5658 5659	CB ASP	729	76. 734 55. 752 56. 420 1. 00 22. 57	A	Č
ATOM	5660	CG ASP	729	76. 819 54. 376 55. 778 1. 00 25. 97	A	č
ATOM	5661	OD1 ASP	729	77. 340 54. 278 54. 649 1. 00 27. 13	Ā	0
ATOM	5662	OD2 ASP	729	76.372 53.388 56.398 1.00 30.03	Α	0 .
ATOM ·	5663	C ASP	729	74.839 56.504 54.984 1.00 19.16	Α	C
ATOM	5664	0 ASP	729	73.868 56.863 55.649 1.00 21.91	Α	0
ATOM	5665	N PHE	730	74.723 55.838 53.846 1.00 18.27	Α	N
ATOM	5666	CA PHE	730	73.416 55.499 53.299 1.00 16.06	Α	C
ATOM	5667	CB PHE	730	72. 796 56. 734 52. 639 1. 00 14. 49	Α	C
ATOM	5668	CG PHE	730	73.590 57.265 51.480 1.00 12.02	A	Č
ATOM	5669	CD1 PHE	730	73. 262 56. 913 50. 177 1. 00 10. 26	A	C
ATOM	5670	CD2 PHE	730	74.691 58.082 51.694 1.00 11.55	A	C
ATOM	5671	CE1 PHE	730	74.020 57.364 49.098 1.00 10.41	Ą	C
ATOM	5672	CE2 PHE	730	75. 459 58. 537 50. 621 1. 00 13. 40	A	C
ATOM	5673	CZ PHE	730	75. 120 58. 175 49. 317 1. 00 9. 85	A	C
ATOM	5674	C PHE	730	73. 565 54. 388 52. 281 1. 00 16. 20	A	C
ATOM	5675	0 PHE	730	74. 675 53. 990 51. 945 1. 00 18. 49	A	0 N
ATOM	5676	N GLN	731	72. 447 53. 883 51. 791 1. 00 17. 40 72. 484 52. 813 50. 813 1. 00 17. 82	A	N C
ATOM	5677	CA GLN	731	101	A A	C
ATOM	5678	CB GLN	731		A	Č
ATOM	5679	CG GLN	731		A	C
ATOM	5680	CD GLN	731		A	Ö
ATOM	5681	OE1 GLN NE2 GLN	731 731	73. 554 49. 883 52. 256 1. 00 32. 85 73. 603 51. 238 54. 055 1. 00 30. 12	A	N
ATOM ATOM	5682 5683		731	72. 091 53. 382 49. 458 1. 00 17. 65	Ä	Ċ
MION	0000	C GUI	(01	12.001 00.002 10.100 1.00 1.00	••	-

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						٠.				(Continued)
					FI	G. 4-	118			(Continued)
ATOM	5733	СВ	ASP	737	70. 884	50. 677	30. 200	1.00 15.90	Α	С
ATOM	5734	CG	ASP	737	72. 232		29. 574	1.00 20.37	Ā	Č
ATOM	5735		ASP	737	72.679		28. 747	1.00 24.29	Ā	Ō
ATOM	5736		ASP	737	72.847		29.895	1.00 18.74	Ā	0
ATOM	5737	C	ASP	737	68.974		31.467	1.00 17.71	Ā	Ċ
ATOM	5738	0	ASP	737	68. 205		30.515	1.00 18.86	Α	0
ATOM	5739	N	GLU	738	68. 553		32.722	1.00 18.39	Ā	N
ATOM	5740	CA	GLU	738	67. 135		33.033	1.00 19.00	Ā	Č
ATOM	5741	CB	GLU	738	66.909		34. 407	1.00 20.24	Ā	Ċ
ATOM	5742	CG	GLU	738	66.904		34. 380	1.00 20.93	A	Ċ
ATOM	5743	CD	GLU	738	65.741		33.565	1.00 24.58	A	C
ATOM	5744		GLU	738	64.588		33.878	1.00 27.21	A	0
ATOM	5745		GLU	738	65.970		32.611	1.00 26.16	A	0
ATOM	5746	C	GLU	738	66.624		33.025	1.00 19.38	Α	C
ATOM	5747	0	GLU	738	67.327		33.461	1.00 20.83	Ā	0
ATOM	5748	N	ASP	739	65.414		32.525	1.00 18.55	Ā	N
ATOM	5749	CA	ASP	739	64.892		32.493	1.00 17.49	Α	С
ATOM	5750	CB	ASP	739	64.074		31.222	1.00 18.32	A	Ċ
ATOM	5751	CG	ASP	739	62. 689			1.00 21.44	Α	C
ATOM	5752	0D1	ASP	739	61.995		30. 257	1.00 24.73	Α	0
ATOM	5753	0D2	ASP	739	62.285		32.358	1.00 21.35	Α	0
ATOM	5754	C	ASP	739	64.088		33.750	1.00 17.35	Α	C
ATOM	5755	0	ASP	739	64. 191	54. 282	34.762	1.00 15.74	Α	0
ATOM	5756	N	HIS	740	63. 291	56.034	33.687	1.00 16.96	Α	N
ATOM	5757	CA	HIS	740	62.521	56.469	34.842	1.00 18.24	Α	С
ATOM	5758	CB	HIS	740	61.746	57. 736	34.511	1.00 16.88	Α	C
ATOM	5759		HIS	740	61.145	58. 392	35.710,	1.00 17.57	Α	C
ATOM	5760		HIS	740	59.883	58. 812	35.961	1.00 16.26	Α	C
ATOM	5761		HIS	740	61.881	58.687	36.837	1.00 17.31	Α	N
ATOM	5762		HIS	740	61.097		37. 732	1.00 18.51	Α	C
ATOM	5763	NE2	HIS	740	59. 880		37. 224	1.00 17.94	Α	N
ATOM	5764	C	HIS	740	61.557		35.426	1.00 19.90	Α	C
ATOM	5765	0	HIS	740	61. 191	55.539	36.599	1.00 20.00	Α	0
ATOM	5766	N	GLY	741	61.151	54. 481	34. 614	1.00 19.40	Α	Ν .
ATOM	5767	CA	GLY	741	60. 216	53. 484	35.084	1.00 18.82	Α	C
ATOM	5768	C	GLY	741	60. 849	52. 218	35.609	1.00 20.36	Α	C
ATOM	5769	0	GLY	741	60. 165	51.404	36.237	1.00 22.79	Α	0
ATOM	5770	N	ILE	742	62. 145	52.045	35. 368	1.00 19.61	Α	N
ATOM	5771	CA	ILE	742	62. 854	50. 849	35. 821	1.00 17.74	Α	C
ATOM	5772	CB	ILE	742	63. 273	50. 981	37. 294	1.00 14.46	Α	C
ATOM	5773		ILE	742	64.279	49. 917	37. 638	1.00 14.37	Α	C
ATOM	5774		ILE	742	63. 865	52.370	37.540	1.00 13.43	Α	C
ATOM	5775		ILE	742	64. 540	52. 552	38. 887	1.00 9.55	A	C .
ATOM	5776	C	ILE	742	61.907	49.658	35.676	1.00 19.11	Α	C
ATOM	5777	0	ILE	742	61.805	48. 825	36. 571	1.00 18.97	Α	0
ATOM	5778	N	ALA	743	61.217	49. 594	34. 534	1.00 20.16	Α	N
ATOM	5779	CA	ALA	743	60. 246	48. 538	34. 268	1.00 19.71	Α	C
ATOM	5780	CB	ALA	743	59.004	49. 141	33. 630	1.00 19.65	A	C
ATOM	5781	C	ALA	743	60. 717	47.350	33. 430	1.00 20.08	Α	С

F I G. 4 - 1 1 9 (Continued)												ntinued)	
ATOM	5782	0	ALA	743	59.8	398	46. 536	33. 006	1.00	20.99	A	0	
ATOM	5783	N	SER	744	62.0		47. 230			19.12	A	N	
ATOM	5784	CA	SER	744	62.4		46.074			17.34	A	C	
ATOM ATOM	5785 5786	CB OG	SER SER	744 744	63. 9 64. 6		46. 132 45. 597			14.62 18.04	A A	C 0	
ATOM	5787	C	SER	744	62. 1		40. 597			16.58	A	C	
ATOM	5788	Õ	SER	744	62. 1		45.032			15.47	A	0	
ATOM	5789	N	SER	745	61.8		43.742			19.10	A	N	
ATOM	5790	CA	SER	745	61.5		42. 558			20.03	A	Č	
ATOM	5791	CB	SER	745	61.4		41.343			20.03	A	Č	
ATOM	5792	OG	SER	745	61.1		40. 209	33. 377		27.90	A	Õ	
ATOM	5793	C	SER	745	62. 5		42. 245	34. 624		19.80	A	Č	
ATOM	5794	. 0	SER	745	62. 1		42.078	35. 781		19.78	A	ŏ	
ATOM	5795	N	THR	746	63. 7		42.158			19.56	A	N	
ATOM	5796	CA	THR	746	64. 7		41.849			19.48	A	Č	
ATOM	5797	CB	THR	746	66. 1		41.538	34. 575		20.06	A	č	
ATOM	5798	0G1	THR	746	66.4		42.615	33. 691		23.41	A	ő	
ATOM	5799		THR	746	66.0		40. 259	33. 772		16. 20	A	Č	
ATOM	5800	C	THR	746	64.9		42.966	36. 288		19.59	A	č	
ATOM	5801	ŏ	THR	746	65.0		42. 706	37. 488		20.63	A	ő	
ATOM	5802	Ň	ALA	747	65.0		44. 208	35. 821		18. 73	A	N	
ATOM	5803	ĊA	ALA	747	65. 2		45. 334	36. 723		18.03	A	Č	
ATOM	5804	CB	ALA	747	65. 5		46.609	35. 919		15.38	A	č	
ATOM	5805	Č	ALA	747	64. 1		45.540	37. 681		17. 35	A	č	
ATOM	5806	0	ALA	747	64. 2		45.989	38. 814		18. 52	Ä	ŏ	
ATOM	5807	N	HIS	748	62. 9		45. 206	37. 224		16.75	Ä	Ň	
ATOM	5808	CA	HIS	748	61.7		45.342	38. 046		16. 92	Ä	Ċ	
ATOM	5809	CB	HIS	748	60.4		45.005	37. 220		13.48	Ä	Č	
ATOM	5810	CG	HIS	748	59. 2		44.968	38. 020		14. 10	- A	Č	
ATOM	5811	CD2	HIS	748	58. 3		43.941	38. 348		12.63	Ā	Č	
ATOM	5812	ND1		748	58.6		46.094	38. 595		14.71	Ä	Ň	
ATOM	5813	CE1	HIS	748	57. 5	61	45.762	39. 241		13.05	A	C	
ATOM	5814	NE2	HIS	748	57. 3	77	44.461	39.107		14.46	A	N	
ATOM	5815	C	HIS	748	61.7	90	44.415	39. 263		18.16	Α	C	
ATOM	5816	0	HIS	748	61.5	25	44.816	40.394	1.00	20.72	Α	0	
ATOM	5817	N	GLN	749	62. 1	48	43.165	39.025	1.00	18.81	A	N	
ATOM	5818	CA	GLN	749	62. 2		42. 201	40.105	1.00	19.53	Α	C	
ATOM	5819	CB	GLN	749	62.4	80	40.801	39. 519	1.00	20.05	A	C	
ATOM	5820		GLN	749	61.2		40.428	38. 550	1.00	21.82	A	C	
ATOM	5821		GLN	749	61.6		39. 190	37. 757	1.00	20.87	Α	С	
ATOM	5822	0E1		749	62.0		38. 187	38. 316		22.37	Α	0	
ATOM	5823	NE2		749	61.4		39. 249	36. 447		20.00	Α	N	
ATOM	5824		GLN	749	63.4		42. 524	41.008		19.07	Α	C	
ATOM	5825		GLN	749	63. 3		42. 388	42. 231		17.88	Α	0	
ATOM	5826		HIS	750	64.5		42.972	40. 399		18.97	Α	N	
ATOM	5827		HIS	750	65.7		43. 275	41.160		16.68	Α	C	
ATOM	5828		HIS	750	66.8		43. 597	40. 226		14.65	A	С	
ATOM	5829		HIS	750	68. 20		43. 496	40.889		13.97	A	С	
ATOM	5830	CD2	HIS	750	69. 20	U7	42. 593	40. 749	1.00	12.94	A	C	

		FIG. 4-121	(Continued)
ATOM 5881 N ATOM 5882 CA ATOM 5883 CB ATOM 5884 OG ATOM 5885 C ATOM 5886 O ATOM 5887 N ATOM 5888 CA ATOM 5889 CB ATOM 5890 CG ATOM 5891 CD2 D ATOM 5893 CE1 D ATOM 5894 NE2 D ATOM 5896 O ATOM 5897 N ATOM 5898 CA ATOM 5898 CA ATOM 5899 CB ATOM 5890 CG ATOM 5891 CD2 D ATOM 5891 CD2 D ATOM 5891 CD2 D ATOM 5895 C ATOM 5896 O ATOM 5897 N ATOM 5898 CA ATOM 5899 CB ATOM 5900 CG ATOM 5901 CD1 D ATOM 5901 CD1 D ATOM 5901 CD1 D ATOM 5901 CD1 D ATOM 5902 CD2 D ATOM 5903 CE1 D ATOM 5905 CZ ATOM 5906 C ATOM 5906 C ATOM 5907 O ATOM 5908 N ATOM 5908 N ATOM 5909 CA ATOM 5911 CG2 D ATOM 5912 CG1 D ATOM 5913 CD1 D ATOM 5914 C ATOM 5915 O ATOM 5916 N ATOM 5917 CA ATOM 5918 CB ATOM 5919 CG ATOM 5920 CD ATOM 5921 CE ATOM 5921 CE ATOM 5921 CE ATOM 5922 NZ ATOM 5923 C ATOM 5924 O ATOM 5925 N ATOM 5925 N ATOM 5925 N ATOM 5926 CA ATOM 5925 N ATOM 5926 CA ATOM	HIS 757 HIS 758 PHE 759 LLE 760 YS 760 LN 761 LN 761 LN 761 LN 761	62. 842	A O O A O C C C C C C C C C C C C C C C

					· F I C	3 1 -	. 1 9 9			(Continued)
ATOM	C000	(ID	OI M	701		3. 4 -				_
ATOM	5929	CD	GLN	761	68. 759	46. 893	58. 283		A	C
ATOM	5930	OE I		761	68. 487	47. 969	57. 739		A	0
ATOM ATOM	5931 5932	NE2	2 GLN GLN	761	69.177	46. 811	59. 544		A	. N
ATOM	5933	C 0	GLN	761 761	65.819	46. 251	58. 701	1.00 32.55	A	C.
ATOM	5934	N	CYS	762	66.064 65.276	46. 149	59.898		A	0
ATOM	5935	CA	CYS	762	64. 945	47. 337 48. 513	58. 161 58. 953	1.00 32.03	A	N C
ATOM	5936	C	CYS	762	63. 888	48. 216	60.023	1.00 33.26 1.00 32.69	A	C
ATOM	5937	ŏ	CYS	762	63. 892	48. 830	61.087	1.00 32.09	A A	C 0
ATOM	5938	ČВ	CYS	762	64. 470	49.643	58. 025	1.00 32.22	A	C
ATOM	5939	SG	CYS	762	63. 606	51.029	58. 843	1.00 40.21	A	S
ATOM	5940	N	PHE	763	62. 993	47. 271	59. 742	1.00 32.59	A	N
ATOM	5941	CA	PHE	763	61.948	46.907	60. 694	1.00 34.25	A	Č
ATOM	5942	CB	PHE	763	60.618	46.647	59. 981	1.00 31.61	A	č
ATOM	5943	CG	PHE	763	59.919	47.892	59. 525	1.00 30.04	Ä	č
ATOM	5944		PHE	763.	60.371	49.148	59.923	1.00 29.45	A	č
ATOM	5945		PHE	763	58.800	47.808	58. 703	1.00 28.65	Ā	Č
ATOM	5946		PHE	763	59. 718	50.300	59.510	1.00 29.27	A	Č
ATOM	5947		PHE	763	58. 139	48. 951	58. 284	1.00 28.76	Α	С
ATOM	5948	CZ	PHE	763	58. 598	50. 202	58.688	1.00 30.54	Α	C C
ATOM	5949	C	PHE	763	62. 293	45.688	61.535	1.00 36.77	Α	C
ATOM	5950	0	PHE	763	61.499	45. 276	62. 381	1.00 36.29	Α	0
ATOM	5951	N	SER	764	63. 463	45. 102	61.290	1.00 39.62	Α	N
ATOM	5952	CA	SER	764	63. 907	43.941	62.052	1.00 43.05	Α	C
ATOM	5953	CB	SER	764 764	65. 356	43. 598	61.701	1.00 44.44	A	C
ATOM ATOM	5954 5955	OG C	SER	764 764	66. 215	44. 709	61.913	1.00 48.06	A	0
ATOM	5956	C 0	SER SER	764	63. 799	44. 314	63. 522	1.00 45.02	A	C
ATOM	5957	N	LEU	764 765	64. 195	45.412	63. 916	1.00 44.75	A	0
ATOM	5958	CA	LEU	765	63. 264 63. 092	43. 412 43. 716	64. 335	1.00 48.04	A	N ·
ATOM	5959	·CB	LEU	765	61.624	44.067	65.747	1.00 51.59 1.00 50.97	A	C
ATOM	5960	CG	LEU	765		44. 846	66. 017 67. 299	1.00 50.97	A	C
ATOM	5961		LEU	765		46. 215	67. 221	1.00 50.79	A	C
ATOM	5962		LEU	765	59. 834	44. 996	67. 481	1.00 50.85	A	C
ATOM	5963	C	LEU	765		42. 588	66. 676	1.00 54.72	A A	C C
ATOM	5964	Ō	LEU	765	62.866	41.557		1.00 55.73	A	0
ATOM	5965	Ň	PRO	766		42.776	67. 372	1.00 57.13	A	N
ATOM	5966	CD	PR ₀	766		43.960	67. 317	1.00 57.88	A	C
ATOM	5967	CA	PRO	766		41.775	68. 301	1.00 58.61	A	C
ATOM	5968	CB	PR0	766		42. 309	68. 604	1.00 58.49	A	č
ATOM	5969	CG	PR0	766		43.797	68. 568	1.00 58.47	A	č
ATOM	5970	С	PR0	766		41.639	69.565	1.00 60.07	Ä	č
ATOM	5971	0	PR0	766		42.370	69.681	1.00 60.04	Ä	Ŏ
ATOM	5972	OXT	PR0	766		40.805	70.427	1.00 61.88	Ä	ŏ
TER	5973		PRO	766					Ä	=
ATOM	5974	CB	ASP	38		45. 132	76.302	1.00 32.66	В	С
ATOM	5975	CG	ASP	38			75.698	1.00 32.61	В	Č
ATOM	5976	0D1		38			75. 977	1.00 30.88	В	0
ATOM	5977	OD2	ASP	38	97. 816	45. 544	74. 942	1.00 31.65	В	0

					FIG	. 4 -	123			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5978 5979 5980 5981 5982 5983 5984 5985 5986 5987 5999 5991 5992 5993 5994 5995 5996 6001 6002 6003 6004 6005 6006 6007 6008	O N CA CB OG C O N CA CB CC CD NE CZ NHI	SER SER SER SER SER SER ARG	38 38 38 39 39 39 39 39 40 40 40 40 40 40 40 41 41 41 41 41 41 41 41 41 41 41 42 42	94. 533 93. 521 94. 842 95. 507 94. 844 93. 974 94. 048 95. 362 94. 289 93. 615 95. 312 95. 685 97. 004 98. 228 99. 470 99. 404 100. 260 101. 247 100. 134 94. 604 93. 881 94. 494 93. 518 93. 386 94. 505 94. 374 93. 307 94. 028 95. 231 93. 118	46. 724 46. 648 44. 428 45. 557 47. 807 48. 982 49. 652 50. 119 50. 017 51. 049 49. 755 50. 257 50. 429 49. 917 48. 479 47. 812 48. 461 46. 497 50. 757 49. 793 51. 907 52. 076 53. 556 54. 209 55. 663 55. 779 54. 922 51. 294 51. 072 50. 859	77. 638 76. 938 78. 423 77. 717 78. 344 78. 372 79. 741 80. 003 77. 220 76. 499 75. 442 74. 788 75. 670 74. 969 74. 728 73. 361 73. 806 74. 376 74. 150 73. 725 72. 658 72. 274 71. 365 69. 840 69. 251 71. 458 71. 324 70. 595	1. 00 31. 81 1. 00 32. 54 1. 00 32. 95 1. 00 32. 06 1. 00 31. 40 1. 00 30. 28 1. 00 34. 53 1. 00 29. 15 1. 00 30. 29 1. 00 26. 40 1. 00 24. 29 1. 00 23. 19 1. 00 21. 38 1. 00 21. 38 1. 00 21. 28 1. 00 22. 73 1. 00 22. 52 1. 00 23. 29 1. 00 24. 31 1. 00 25. 29 1. 00 28. 84 1. 00 28. 84 1. 00 28. 95 1. 00 24. 69 1. 00 23. 54 1. 00 23. 54 1. 00 24. 69 1. 00 23. 54 1. 00 23. 54	B B B B B B B B B B B B B B B B B B B	
ATOM ATOM ATOM ATOM	6009 6010 6011 6012	CB OG1	THR THR THR THR	42 42 42 42	92. 454 91. 257	50. 130 49. 083 49. 753 48. 129	69. 399 68. 959 68. 540 70. 101	1.00 22.29 1.00 22.69 1.00 21.91 1.00 20.28	B B B	C C O C
ATOM ATOM ATOM ATOM ATOM	6013 6014 6015 6016 6017	C O N CA CB	THR THR TYR TYR TYR	42 42 43 43 43	93. 641 93. 386 94. 045 94. 158 95. 233	51. 178 52. 363 50. 750 51. 662 51. 153	68. 304 68. 541 67. 116 65. 986 65. 020	1. 00 22. 33 1. 00 23. 36 1. 00 20. 55 1. 00 19. 19 1. 00 20. 32	B B B B	C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6018 6019 6020 6021 6022 6023 6024 6025 6026	CE1 CD2	TYR	43 43 43 43 43 43 43 43	94. 888 95. 133 96. 403 96. 655 96. 013 96. 247 92. 770	53. 126		1.00 19.92 1.00 22.19 1.00 21.23 1.00 21.09 1.00 21.69 1.00 22.25 1.00 25.44 1.00 18.52 1.00 17.41	B B B B B B	C C C C C C C C C C C C C C C C C C C

					FIC	G. 4-	124			(Continued)
ATOM	6027	N	THR	44	92.007	52.709	65.532	1.00 17.70	В	N
ATOM	6028	CA	THR	44	90.633	52.802	65.019	1.00 18.55	В	C
ATOM	6029	CB	THR	44	89.762	53. 748	65.877	1.00 16.45	В	С
ATOM	6030	0G1	THR	44	90. 195	55.096	65.676	1.00 16.93	В	0
ATOM	6031	CG2	THR	44	89. 875	53.409	67.346	1.00 14.45	В	C
ATOM	6032	C	THR	44	90. 521	53.310	63.593	1.00 19.62	В	C
ATOM	6033	0	THR	44	91.511	53. 741	62.992	1.00 21.89	В	0
ATOM	6034	N	LEU	45	89. 296	53. 277	63.067	1.00 19.06	В	N
ATOM	6035	CA	LEU	45	89.026	53.749	61.713	1.00 18.74	В	C
ATOM	6036	CB	LEU	45	87.570	53.489	61.327	1.00 17.33	В	С
ATOM	6037	CG	LEU	45	87. 163	54.032	59.952	1.00 17.35	В	C C
ATOM	6038		LEU	45	88. 050	53.417	58.873	1.00 15.87	В	С
ATOM	6039		LEU	45	85.698	53.720	59.681	1.00 16.27	В	C
ATOM	6040	C	LEU	45	89. 300	55. 240	61.638	1.00 19.82	В	C
ATOM	6041	0	LEU	45	89. 827	55. 743	60. 638	1.00 21.32	В	0
ATOM	6042	N	THR	46	88. 948	55. 945	62. 707	1.00 19.07	В	N
ATOM	6043	CA	THR	46	89. 156	57. 382	62.760	1.00 20.55	В	C
ATOM	6044	CB	THR	46	88. 550	57.988	64.038	1.00 21.32	В	C
ATOM	6045	0G1		46	87. 148	57.700	64.083	1.00 21.56	В	0
ATOM	6046	CG2		46	88. 745	59.497	64.053	1.00 20.61	В	С
ATOM	6047	C	THR	46	90.634	57. 749	62.694	1.00 21.16	В	C
ATOM	6048	0	THR	46	90. 999	58. 759	62.092	1.00 21.06	В	0
ATOM	6049	N	ASP	47	91. 491	56.945	63. 313	1.00 21.00	В	N
ATOM	6050	CA	ASP	47	92. 910	57. 253	63. 262	1.00 22.97	В	C
ATOM	6051	CB	ASP	47	93. 731	56. 273	64.110	1.00 25.34	В	C
ATOM	6052	CG	ASP	47	93. 365	56.322	65. 578	1.00 27.23	В	C
ATOM	6053	0D1		47	93. 116	57. 430	66. 105	1.00 26.32	В	0
ATOM	6054	OD2		47	93. 339	55. 244	66. 208	1.00 31.41	В	0
ATOM	6055	C	ASP	47	93. 357	57.178	61.810	1.00 22.85	В	C
MOTA	6056	0	ASP	47	94. 057	58.065	61.320	1.00 24.15	В	0
ATOM	6057	N	TYR	48	92. 951	56. 124	61.114	1.00 20.92	В	N
ATOM	6058	CA	TYR	48	93. 332	55.998	59. 720	1.00 21.40	В	C
ATOM	6059	CB	TYR	48	92. 823	54.676	59. 136	1.00 19.45	В	C
ATOM	6060	CCC	TYR TYR	48	92.867	54.612	57.624	1.00 18.60	В	C
ATOM ATOM	6061 6062	CE1		48	94.062	54. 787	56. 927	1.00 18.00	В	C
ATOM	6063		TYR	48 48	94. 098			1.00 16.57	В	C
ATOM	6064		TYR	48 48	91.702	54. 383	56. 885	1.00 21.30	В	C
ATOM	6065	CZ	TYR	46 48	91.726	54. 329	55. 489 54. 822	1.00 19.50	В	C
ATOM	6066	OH	TYR	48	92. 925	54. 503		1.00 18.43	В	C
ATOM	6067	C	TYR	48	92. 942 92. 795	54. 434 57. 170	53. 452 58. 899	1.00 18.40 1.00 21.85	В	0
ATOM	6068	Õ	TYR	48	93. 547	57. 853	58. 207	1.00 21.85	В	C
ATOM	6069	N	LEU	49	91. 497	57.416	58. 996	1.00 21.92	B B	0 N
ATOM	6070		LEU	49	90. 885	58. 485	58. 223	1.00 25.08	В	N C
ATOM	6071		LEU	49	89. 359	58. 437	58. 381	1.00 28.14	В	C
ATOM	6072		LEU	49	88. 688	57. 157	57. 872	1.00 28.75	В	Č
ATOM	6073	CD1		49	87. 188	57. 305	57. 980	1.00 28.73	В	C
ATOM	6074	CD2		49	89. 094	56. 889	56. 420	1.00 28.45	В	C
ATOM	6075		LEU	49	91.391	59. 886	58. 544	1.00 28.33	В	Č

			•		(Continued)
				FIG. 4-126	
ATOM	6125		55	104. 959 58. 926 59. 515 1. 00 24. 45 B	С
ATOM	6126		55	105. 025 57. 911 58. 382 1. 00 22. 51 B	
ATOM	6127		55	104. 335 56. 575 58. 631 1. 00 23. 77 B	
MOTA	6128		55	104. 287 55. 792 57. 336 1. 00 23. 51 B	
ATOM ATOM	6129 6130		55	105. 083 55. 796 59. 703 1. 00 22. 83 B	
ATOM	6131		55 56	105. 773 60. 161 59. 135 1. 00 24. 19 B	
ATOM	6132		55 56	105. 428 60. 867 58. 187 1. 00 23. 47 B 106. 824 60. 456 59. 886 1. 00 23. 25 B	
ATOM	6133		56	108 004 01 000 00	
ATOM	6134		56	100 500 00 500	
ATOM	6135		56	108. 536 62. 028 60. 680 1. 00 25. 76 B 107. 850 62. 922 61. 697 1. 00 29. 15 B	
ATOM	6136		56	108. 868 63. 560 62. 638 1. 00 31. 22 B	C C
ATOM	6137	CE LYS	56	108. 225 64. 593 63. 548 1. 00 32. 59 B	C
ATOM	6138		56	109. 235 65. 233 64. 439 1. 00 34. 54 B	N
ATOM	6139	C LYS	56	108. 458 61. 196 58. 330 1. 00 23. 35 B	Č
ATOM	6140	0 LYS	56	108. 833 60. 035 58. 186 1. 00 23. 24 B	ŏ
ATOM	6141	N LEU	57	108.717 62.162 57.462 1.00 22.99 B	N
ATOM	6142	CA LEU	57	109.477 61.945 56.247 1.00 22.29 B	Ċ
ATOM	6143	CB LEU	57	108. 612 62. 292 55. 040 1. 00 23. 21 B	Č
ATOM	6144	CG LEU	57	107. 169 61. 794 55. 037 1. 00 23. 82 B	С
ATOM	6145	CD1 LEU	57 57	106. 440 62. 380 53. 841 1. 00 24. 84 B	C
ATOM Atom	6146 6147	CD2 LEU	57	107.145 60.278 54.992 1.00 25.36 B	C
ATOM	6148	C LEU O LEU	57	110. 681 62. 870 56. 256 1. 00 22. 04 B	С
ATOM	6149	O LEU N TYR	57 50	110. 888 63. 628 57. 202 1. 00 22. 65 B	0
ATOM	6150	CA TYR	58 58	111.468 62.809 55.191 1.00 20.44 B 112.624 63.674 55.065 1.00 20.14 B	N
ATOM	6151	CB TYR	58	110 001 00 000	C
ATOM	6152	CG TYR	58	114 000 04 000 70 000	C
ATOM	6153	CD1 TYR	58	115 045 04 000 54 000	C
ATOM	6154	CE1 TYR	58	115.845 64.392 54.998 1.00 19.13 B 116.816 65.380 55.165 1.00 18.92 B	C C
ATOM	6155	CD2 TYR	58	115. 022 64. 816 57. 201 1. 00 19. 88 B	C
ATOM	6156	CE2 TYR	58	115. 987 65. 807 57. 378 1. 00 19. 69 B	Č
ATOM	6157	CZ TYR	58	116.877 66.086 56.355 1.00 19.43 B	Č
ATOM	6158	OH TYR	58	117.804 67.092 56.508 1.00 19.58 B	ŏ
ATOM	6159	C TYR	58	112. 917 63. 819 53. 590 1. 00 20. 38 B	Č
ATOM	6160	O TYR	58	113.861 63.223 53.079 1.00 20.32 B	0
ATOM	6161		59	112.085 64.604 52.909 1.00 21.33 B	N
ATOM ATOM	6162	CA SER	59 50	112. 245 64. 839 51. 479 1. 00 22. 11 B	C
ATOM	6163 6164	CB SER OG SER	59	110. 920 65. 275 50. 852 1. 00 21. 08 B	C
ATOM	6165	C SER	59	109. 985 64. 212 50. 843 1. 00 24. 94 B	0
ATOM	6166	0 SER	59 59	113. 293 65. 895 51. 191 1. 00 21. 64 B 113. 099 67. 064 51. 491 1. 00 23. 87 B	Ç.
ATOM	6167	N LEU	60	114 404 0= 115	0
ATOM	6168	CA LEU	60	115 110	N C
ATOM	6169	CB LEU	60	110 770	C
ATOM	6170	CG LEU	60	116. 752 66. 062 50. 986 1. 00 22. 27 B 117. 406 64. 737 50. 612 1. 00 18. 62 B	C
ATOM	6171	CD1 LEU	60	118.176 64.900 49.320 1.00 17.05 B	C C
ATOM	6172	CD2 LEU	60	118.338 64.313 51.724 1.00 19.95 B	C
ATOM	6173	C LEU	60	115.656 66.478 48.762 1.00 24.93 B	Č
				SUBSTITUTE SHEET (RULE 26)	•

										(Continued)
					FIC	G. 4-	127			
ATOM	6174	0	LEU	60	115.176	65. 604	48.029	1.00 23.79	В	0
ATOM	6175		ARG	61	116.375	67. 495	48. 302	1.00 26.02	В	N
ATOM	6176		ARG	61	116.634	67. 659	46.881	1.00 27.11	В	C
ATOM	6177		ARG	61	115.693	68. 728	46. 329	1.00 32.13	В	C
ATOM ATOM	6178 6179		ARG ARG	61 61	115. 779 115. 002	68. 979 70. 243	44. 833 44. 495	1.00 38.27 1.00 41.78	B B	C C
ATOM	6180		ARG	61	114. 937	70. 506	43.063	1.00 41.78	В	N
ATOM	6181		ARG	61	114. 298	71. 543	42.525	1.00 49.47	В	Č
ATOM	6182	NH1		61	113.671	72. 420	43. 307	1.00 48.74	B	Ň
ATOM	6183	NH2		61	114. 266	71.693	41.205	1.00 50.07	В	N
ATOM	6184		ARG	61	118.080	68.075	46.676	1.00 26.01	В	С
ATOM	6185		ARG	61	118.475	69. 180	47.052	1.00 26.36	В	0
ATOM	6186		TRP	62	118.877	67. 186	46.095	1.00 25.15	В	Ň
ATOM	6187		TRP	62	120. 282	67. 488	45.846	1.00 24.48	В	C
ATOM ATOM	6188 6189		TRP TRP	62 62	121.024	66. 244 65. 145	45. 355 46. 365	1.00 20.04 1.00 18.16	В	C C
ATOM	6190	CD2		62	121.095 121.954	65. 092	40. 503	1.00 16.10	B B	C
ATOM	6191	CE2		62	121.639	63. 910	48. 215	1.00 15.18	В	Č
ATOM	6192	CE3		62	122. 956	65. 932	48.007	1.00 12.41	B	č
ATOM	6193	CD1		62	120.315	64.017	46.419	1.00 17.39	B	Č
ATOM	6194	NE1		62	120.639	63. 272	47. 528	1.00 15.77	В	N
ATOM	6195	CZ2		62	122. 292	63. 546	49. 397	1.00 16.35	В	С
ATOM	6196	CZ3		62	123.606	65. 575	49. 183	1.00 14.94	В	C
ATOM	6197	CH2		62	123. 271	64. 389	49.866	1.00 16.25	В	C
ATOM ATOM	6198 6199		TRP TRP	62 62	120. 401 119. 863	68. 588 68. 457	44. 798 43. 698	1.00 26.73 1.00 27.86	В	C
ATOM	6200		ILE	63	121.088	69. 675	45. 135	1.00 27.80	B B	O N
ATOM	6201		ILE	63	121. 265	70. 763	44. 180	1.00 21.37	В	Č
ATOM	6202		ILE	63	120. 947	72. 130	44. 803	1.00 29.64	B	č
ATOM	6203	CG2		63	119.476	72.193	45.169	1.00 30.36	B	Č
ATOM	6204	CG1		63	121.830	72.372	46.027	1.00 30.01	В	C
ATOM	6205	CD1		63	121.542	73.682	46. 736	1.00 27.88	В	C
ATOM	6206		ILE	63	122.693	70.771	43.657	1.00 30.19	В	C
ATOM ATOM	6207 6208		ILE SER	63	123.062	71.609	42. 835	1.00 31.12	В	0
ATOM	6209		SER	64 64	123. 485 124. 876	69.816	44.132	1.00 30.03 1.00 30.53	В	N
ATOM	6210		SER	64	124. 870	70. 808	43. 718	1.00 30.33	B B	C C
ATOM	6211		SER	64	125. 848	70. 724	45. 679	1.00 27.92	В	Õ
ATOM	6212		SER	64	125. 399	68. 343	44. 255	1.00 31.08	В	Č
ATOM	6213		SER	64	124. 630	67. 488	44. 691	1.00 31.36	B	Ö
ATOM	6214		ASP	65	126. 712	68.176	44. 236	1.00 31.42	В	N
ATOM	6215		ASP	65	127. 306	66.947	44. 728	1.00 32.55	В	C
ATOM	6216		ASP	65	128. 576	66. 633	43. 945	1.00 33.28	В	C
ATOM	6217		ASP	65 65	129. 158	65. 286	44. 302	1.00 35.12	В	C
ATOM ATOM	6218 6219	0D1 A		65 65	128. 446	64. 261	44. 158	1.00 33.02	В	0
ATOM	6220	OD2 A	asp ASP	65 65	130. 331 127. 636	65. 259	44. 728	1.00 37.02 1.00 32.66	В	0
ATOM	6221		asp ASP	65	127.030	67. 045 66. 069	46. 211 46. 818	1.00 32.00	B B	C 0
ATOM	6222		HIS	66	127. 399	68. 217	46. 796	1.00 33.06	В	N N
	**	•				30. 211	20. 100		,	41

					D. I. C	, À	1.00			(Continued)
					FIG	3.4-	128			
ATOM	6223	CA	HIS	66	127.704	68.440	48. 203	1.00 32.64	В	C
ATOM	6224	CB	HIS	66	128. 892	69. 402	48. 329	1.00 35.63	В	C
ATOM	6225	CG	HIS	66	130.032	69.076	47. 416	1.00 39.09	В	C
ATOM	6226		HIS	66 66	131.260	68. 562	47.669	1.00 40.29	В	C
ATOM	6227 6228		HIS HIS	66 66	129. 959 131. 092	69. 238 68. 835	46. 047 45. 498	1.00 41.80 1.00 42.37	B B	N C
ATOM ATOM	6229		HIS	66	131. 092	68. 420	46. 459	1.00 42.31	В	N N
ATOM	6230	C	HIS	66	126. 547	69.001	49.016	1.00 31.01	В	Ċ
ATOM	6231	ŏ	HIS	66	126.602	69.008	50. 245	1.00 30.92	B	ŏ
ATOM	6232	Ň	GLU	67	125. 505	69. 479	48. 345	1.00 30.05	B	N
ATOM	6233	CA	GLU	67	124.379	70.067	49.062	1.00 28.07	В	C
ATOM	6234	CB	GLU	67	124.457	71.591	48. 984	1.00 27.21	В	C
ATOM	6235	CG	GLU	67	125.601	72. 179	49. 781	1.00 29.99	В	Č
ATOM	6236	CD	GLU	67	125. 745	73.675	49.593	1.00 32.09	В	C
ATOM	6237		GLU	67	126. 408	74. 315	50.438	1.00 33.25	В	0
ATOM ATOM	6238 6239	C	GLU GLU	67 67	125. 207 123. 015	74. 209 69. 619	48. 599 48. 583	1.00 34.83 1.00 27.52	В В	0 C
ATOM	6240	0	GLU	67	123. 013	69. 085	47. 482	1.00 27.32	В	0 .
ATOM	6241	Ň	TYR	68	122.012	69.855	49.425	1.00 26.72	В	N
ATOM	6242	CA	TYR	68	120. 634	69. 498	49.116	1.00 25.74	B	Ĉ
ATOM	6243	CB	TYR	68	120. 347	68.069	49. 592	1.00 23.47	B	Č
ATOM	6244		TYR	68	120.373	67.847	51.094	1.00 22.93	В	C
ATOM	6245		TYR	68	119. 339	68. 319	51.914	1.00 22.75	В	C
ATOM	6246		TYR	68	119.312	68.040	53. 282	1.00 21.24	В	C
ATOM	6247		TYR	68	121.391	67.097	51.685	1.00 22.05	В	C
ATOM	6248		TYR	68	121.379	66.812	53.053	1.00 22.38	В	C
ATOM ATOM	6249 6250	CZ OH	TYR TYR	68 68	120. 333 120. 300	67. 283 66. 973	53. 847 55. 191	1.00 23.05 1.00 18.34	B B	C 0
ATOM	6251	C	TYR	68	119.657	70. 481	49. 759	1.00 16.34	В	C.
ATOM	6252	ŏ	TYR	68	119.961	71.077	50. 789	1.00 26.50	В	Õ
ATOM	6253	Ň	LEU	69	118. 497	70. 674	49. 139	1.00 26.72	B	Ň
ATOM	6254	CA	LEU	69	117.492	71.580	49.694	1.00 27.89	B	Ċ
ATOM	6255	CB	LEU	69	116.729	72.316	48.586	1.00 24.29	В	C
ATOM	6256	CG	LEU	69	117. 545	73. 257	47.695	1.00 23.81	В	C
ATOM	6257		LEU	69	116.656	73. 891	46.633	1.00 19.95	В	C
ATOM	6258		LEU	69	118. 187	74. 324	48. 552	1.00 24.79	В	C
ATOM	6259	C	LEU	69	116.508	70.777	50. 543	1.00 29.18	В	C
ATOM ATOM	6260 6261	O N	LEU TYR	69 70	116. 226 115. 998	69.609 71.411	50. 260 51. 590	1.00 28.86 1.00 29.78	B B	0
ATOM	6262	CA	TYR	70 .	115. 956	70. 765	52. 482	1.00 29.78	В	N C
ATOM	6263	CB	TYR	70	115. 799	70. 142	53. 667	1.00 31.46	В	C
ATOM	6264	ĊĠ	TYR	70	114.910	69. 348	54. 592	1.00 26.47	B	č
ATOM	6265	CD1	TYR	70	114. 396	68.114	54. 206	1.00 25.75	B	č
ATOM	6266	CE1	TYR	70	113. 544	67.398	55.038	1.00 26.40	В	Č
ATOM	6267		TYR	70	114.553	69.847	55.842	1.00 28.33	В	C
ATOM	6268			70	113. 701	69. 141	56.686	1.00 28.03	В	Č
ATOM	6269	CZ	TYR	70	113. 199	67.918	56. 276	1.00 28.21	В	C
ATOM ATOM	6270 6271	OH C	TYR TYR	70 70	112. 346	67. 221	57. 103	1.00 30.20	В	0
MIOM	04(1	U	ли	70	114.056	71. 796	52. 983	1.00 34.45	В	C

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										(Continued)
					FIG	4 -	130			
ATOM 6 AT	324 325 326 327 328 3329 3331 3333 3334 3335 3336 3336 3337 6340 6342 6344 6345 6346 6347 6346 6347 6351 6352 6353 6353	O N I I CA I CB I CCD2 I CCD2 C C O N CA CB CCD1 CCD2 CC C C CCD1 CCD2 CC CCD1 CCD2 CCC CCCCCC CCCCCCCCCC	ILE ILEU LEU LEU LEU LEU LEU LEU LEU LEU LEU	76 76 76 77 77 77 77 77 77 77 77 78 78 78 78 79 79 79 79 79 79 79 79 79 80 80 80 80 80 80	112. 341 115. 243 115. 758 115. 862 117. 208 117. 227 116. 155 116. 435 116. 149 118. 121 117. 657 119. 417 120. 409 121. 227 120. 311 121. 346 121. 781 121. 660 122. 530 121. 807 120. 680 119. 499 120. 789 118. 448 119. 749 118. 573 123. 841 124. 876 125. 174 127. 276 128. 653 128. 916	77. 009 76. 589 77. 701 75. 472 75. 498 74. 901 75. 359 74. 728 76. 874 74. 683 73. 821 74. 967 74. 253 75. 227 74. 480 75. 906 73. 523 74. 087 72. 272 71. 496 70. 247 70. 531 71. 120 70. 168 71. 338 70. 382 70. 967 71. 036 70. 729 70. 992 70. 518 71. 307 70. 689 69. 567 71. 421	48. 967 53. 043 53. 150 53. 400 53. 941 55. 351 56. 346 57. 701 56. 460 53. 036 52. 289 53. 103 52. 308 51. 431 50. 691 50. 448 53. 263 54. 261 52. 956 53. 821	1. 00 42. 01 1. 00 39. 85 1. 00 41. 15 1. 00 36. 42 1. 00 34. 28 1. 00 34. 54 1. 00 33. 23 1. 00 34. 45 1. 00 32. 91 1. 00 30. 72 1. 00 30. 72 1. 00 30. 20 1. 00 29. 01 1. 00 31. 37 1. 00 28. 37 1. 00 28. 37 1. 00 28. 37 1. 00 28. 37 1. 00 28. 38 1. 00 26. 51 1. 00 24. 85 1. 00 24. 45 1. 00 22. 62 1. 00 20. 15 1. 00 19. 84 1. 00 20. 35 1. 00 16. 96 1. 00 18. 97 1. 00 24. 95 1. 00 24. 95 1. 00 24. 94 1. 00 23. 66 1. 00 23. 32 1. 00 22. 91 1. 00 22. 91 1. 00 23. 26 1. 00 21. 99	B B B B B B B B B B B B B B B B B B B	Continued) C C C C C C C C C C C C C C C C C C
ATOM ATOM	6355 6356 6357	0	ASN ASN	80 80 80	129. 542 126. 156 126. 168	69. 077 68. 842		1.00 21.99 1.00 24.17 1.00 25.80 1.00 23.17	В В В	N C O N
ATOM ATOM	6358 6359 6360	CB	ALA ALA	81 81 81	126. 116 126. 054 126. 025	68. 116 66. 713 65. 819 66. 256	53. 496 52. 246 54. 434	1.00 23.17 1.00 24.07 1.00 20.69 1.00 25.23	В В В	C C C
ATOM ATOM ATOM	6361 6362 6363 6364	C O N CA	ALA ALA GLU GLU	81 81 82 82	127. 167 126. 925 128. 377 129. 525	65. 462 66. 764 66. 351	55. 347 54. 222 55. 024	1.00 25.26 1.00 26.73 1.00 29.51	В В В	O N C
ATOM ATOM ATOM ATOM	6365 6366 6367 6368 6369	CB CG CD OE1	GLU GLU GLU GLU GLU	82 82 82 82 82	130. 820 132. 124 132. 287 132. 064 132. 659	66. 835 66. 326 64. 800 64. 191 64. 209	54. 361 55. 005 54. 955 53. 884 55. 995	1.00 32.02 1.00 35.72 1.00 38.90 1.00 38.71 1.00 40.81	B B B B	C C O O

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										(Continued)
					FIC	G. 4-	131			(001111111000)
ATOM	6370	С	GLU	82	129. 528	66. 757	56. 497	1.00 29.17	В	С
ATOM	6371	0	GLU	82	130. 102	66.051	57.324	1.00 28.55	В	0
ATOM	6372	N	TYR	83	128.888		56.834	1.00 29.07	В	N
ATOM	6373	CA	TYR	83	128. 877	68. 329	58. 223	1.00 28.95	В	С
ATOM	6374	CB	TYR	83	129. 504		58. 320	1.00 30.17	В	C
ATOM	6375	CG	TYR	83	130. 821	69. 834	57. 596	1.00 33.40	В	C
ATOM	6376		TYR	83	131.914	69. 049	57.963	1.00 33.79	В	C
ATOM	6377		TYR	83	133. 120	69. 129	57. 271	1.00 36.07	В	C
ATOM	6378		TYR	83	130.966	70. 704	56.517	1.00 35.97	В	C
ATOM	6379		TYR	83	132.162	70. 791	55.815	1.00 36.91	В	C
ATOM ATOM	6380 6381	CZ OH	TYR TYR	83 83	133. 234 134. 413	70. 003 70. 091	56.195	1.00 38.12	В	C
ATOM	6382	C	TYR	83	127. 490	68. 355	55. 486 58. 853	1.00 42.42 1.00 28.16	B B	0 C
ATOM	6383	0	TYR	83	127. 430	68. 093	60.044	1.00 28.10	В	0
ATOM	6384	N	GLY	84	126.478	68. 684	58.063	1.00 25.04	В	N N
ATOM	6385	CA	GLY	84	125. 136	68. 726	58. 601	1.00 24.77	В	Č
ATOM	6386	C	GLY	84	124.668	70. 137	58. 880	1.00 24.11	В	Č
ATOM	6387	ŏ	GLY	84	123. 511	70. 345	59. 222	1.00 23.68	В	ŏ
ATOM	6388	N	ASN	85	125. 565	71. 109	58. 745	1.00 26.40	B	Ň
ATOM	6389	CA	ASN	85	125. 201	72.501	58. 984	1.00 27.79	B	Ċ
ATOM	6390	CB	ASN	85	126.446	73.366	59. 181	1.00 28.01	B	Č
ATOM	6391	CG	ASN	85	127.356	73.363	57.975	1.00 31.32	В	Č
ATOM	6392	OD1	ASN	85	128.051	72.384	57.697	1.00 31.73	В	0
ATOM	6393		ASN	85	127. 338	74.472	57. 250	1.00 33.71	В	Ň
ATOM	6394	C	ASN	85	124. 381	73.023	57.813	1.00 28.62	В	C
ATOM	6395	0	ASN	85	124. 432	72.472	56.720	1.00 28.74	В	0
ATOM	6396	N	SER	86	123.622	74.085	58.043	1.00 30.17	В	N
ATOM	6397	CA	SER	86	122. 787	74.633	56. 991	1.00 32.38	В	C
ATOM	6398	CB	SER	86	121.392	74.005	57.061	1.00 31.71	В	С
ATOM	6399	OG	SER	86	120.734	74.380	58. 256	1.00 32.32	В	0
ATOM	6400	C	SER	86 86	122.658	76.145	57.063	1.00 33.63	В	C
ATOM ATOM	6401 6402	0 N	SER	86	123. 307	76.800	57. 874	1.00 34.72	В	0
ATOM	6403	N CA	SER SER	87 87	121.806	76.682	56. 195	1.00 35.45	В	N
ATOM	6404	CB	SER	87	121.530 122.588	78.111	56. 115	1.00 35.95	В	C
ATOM	6405	OG	SER	87	122. 366	78. 825 78. 635	55. 280 55. 810	1.00 35.50	B B	C
ATOM	6406	C	SER	87	120. 191	78. 233	55. 418	1.00 39.27 1.00 36.74	_	0
ATOM	6407	ŏ	SER	87	119. 832	77. 369	54. 625	1.00 30.74	B B	C
ATOM	6408	Ň	VAL	88	119.444	79. 288	55. 723	1.00 38.47	В	O N
ATOM	6409	ĊA	VAL	88	118. 154	79. 498	55. 084	1.00 36.32	В	C
ATOM	6410	CB	VAL	88	117. 357	80.636	55. 750	1.00 37.21	В	Č
ATOM	6411	CG1		88	116.094	80.916	54. 954	1.00 36.84	В	Č
ATOM	6412	CG2		88	117.006	80. 260	57. 186	1.00 38.04	В	Č
ATOM	6413	С	VAL	88	118. 422	79.897	53. 647	1.00 36.83	B	č
ATOM	6414	0	VAL	88	119. 235	80. 782	53. 379	1.00 36.34	B	ŏ
ATOM	6415		PHE	89	117. 745	79. 240	52.719	1.00 36.53	B	Ň
ATOM	6416		PHE	89	117. 925	79.552	51.314	1.00 37.05	B	Ċ
ATOM	6417		PHE	89	117. 901	78. 262	50. 491	1.00 34.62	В	Č
ATOM	6418	CG	PHE	89	118.060	78. 474	49.014	1.00 31.67	В	С
				_				_		

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		FIG. 4-132	(Continued)
ATOM 6419 CD1 PHE ATOM 6420 CD2 PHE ATOM 6421 CE1 PHE ATOM 6422 CE2 PHE ATOM 6423 CZ PHE ATOM 6424 C PHE ATOM 6425 O PHE ATOM 6426 N LEU ATOM 6427 CA LEU ATOM 6428 CB LEU ATOM 6429 CG LEU ATOM 6430 CD1 LEU ATOM 6431 CD2 LEU ATOM 6431 CD2 LEU ATOM 6432 C LEU ATOM 6433 O LEU ATOM 6434 N GLU ATOM 6435 CA GLU ATOM 6436 CB GLU ATOM 6437 CG GLU ATOM 6438 CD GLU ATOM 6439 OE1 GLU ATOM 6439 OE1 GLU ATOM 6440 OE2 GLU ATOM 6441 C GLU ATOM 6441 C GLU ATOM 6442 O GLU ATOM 6443 N ASN ATOM 6444 CA ASN ATOM 6445 CB ASN ATOM 6445 CB ASN ATOM 6446 CG ASN ATOM 6447 OD1 ASN ATOM 6448 ND2 ASN ATOM 6449 C ASN ATOM 6449 C ASN ATOM 6445 CB SER ATOM 6450 O ASN ATOM 6451 N SER ATOM 6452 CA SER ATOM 6454 OG SER ATOM 6454 OG SER ATOM 6456 O SER ATOM 6457 N THR ATOM 6458 CA THR ATOM 6459 CB THR ATOM 6450 CG THR ATOM 6450 CG THR ATOM 6451 CG THR	89 89 89 89 89 90 90 90 90 91 91 91 91 91 92 92 92 92 92 93 93 93 94 94 94 94 94	116. 963 78. 790 48. 223 1. 00 29. 04 119. 303 78. 333 48. 412 1. 00 31. 62 117. 095 78. 968 46. 857 1. 00 28. 72 119. 450 78. 500 47. 038 1. 00 32. 27 118. 342 78. 813 46. 258 1. 00 39. 38 116. 801 80. 483 50. 896 1. 00 39. 89 115. 733 80. 493 51. 688 1. 00 41. 53 114. 581 81. 332 51. 403 1. 00 43. 78 113. 849 80. 788 50. 173 1. 00 44. 69 112. 818 81. 664 49. 462 1. 00 44. 94 113. 439 83. 000 49. 088 1. 00 44. 39 112. 328 80. 944 48. 217 1. 00 44. 54 113. 192 80. 302 53. 062 1. 00 45. 79 113. 192 80. 302 53. 062 1. 00 45. 79 113. 192 80. 302 53. 062 1. 00 44. 77 113. 395 82. 542 53. 140 1. 00 49. 59 112. 524 82. 715 54. 302 1. 00 51. 78 112. 524 82	B C C C C C C C C C C C C C C C C C O N C C C C
ATOM 6463 C THR ATOM 6463 O THR ATOM 6464 N PHE ATOM 6465 CA PHE ATOM 6466 CB PHE ATOM 6467 CG PHE	94 94 95 95 95	108. 330 86. 418 50. 689 1. 00 54. 94 B 108. 424 87. 339 49. 878 1. 00 55. 42 B 107. 256 85. 640 50. 762 1. 00 54. 35 B 106. 125 85. 865 49. 873 1. 00 54. 57 B 105. 956 84. 681 48. 914 1. 00 53. 35 B 107. 158 84. 426 48. 043 1. 00 52. 21 B	C O N C C C

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						(Continued)
				FIG. 4-133		(Continued)
ATOM	6468	CD1 PHE	95		1.00 51.86 B	C
ATOM	6469	CD2 PHE	95		1.00 51.89 B	C
ATOM	6470	CE1 PHE	95		1.00 50.37 B	C C
ATOM	6471	CE2 PHE	95 05		1.00 51.43 B	C
ATOM	6472	CZ PHE C PHE	95 95		I.00 50.62 B	C
ATOM ATOM	6473 6474	0 PHE	95 95		1.00 55.16 B	Ö
ATOM	6475	N ASP	96		1.00 56.69 B	Ň
ATOM	6476	CA ASP	96		1.00 57.24 B	Ċ
ATOM	6477	CB ASP	96		.00 58.96 B	č
ATOM	6478	CG ASP	96		. 00 60. 91 B	Č
ATOM	6479	OD1 ASP	96		.00 60.82 B	0
ATOM	6480	OD2 ASP	96		.00 62.59 B	0
ATOM	6481	C ASP	96		.00 57.24 B	C
ATOM	6482	0 ASP	96	101.498 87.401 52.100 1	.00 58.26 B	0
ATOM	6483	N GLU	97		1.00 57.07 B	N
ATOM	6484	CA GLU	97		L.00 57.68 B	C
ATOM	6485	CB GLU	97		. 00 59. 15 B	C
ATOM	6486	CG GLU	97		.00 61.76 B	Č
ATOM	6487	CD GLU	97		. 00 63. 57 B	C
ATOM	6488	OE1 GLU	97		. 00 63. 88 B	0
ATOM	6489	OE2 GLU	97		. 00 64. 73 B	0
ATOM	6490	C GLU	97		. 00 56. 86 B	C
ATOM ATOM	6491 6492	O GLU N PHE	97		.00 58.05 B	0 N
ATOM	6493	N PHE CA PHE	98 98		. 00 54. 75 B . 00 52. 58 B	N C
ATOM	6494	CB PHE	98		.00 52.56 B	C C
ATOM	6495	CG PHE	98		.00 51.74 B	C
ATOM	6496	CD1 PHE	98		.00 50.75 B	Č
ATOM	6497	CD2 PHE	98		.00 51.54 B	č
ATOM	6498	CE1 PHE	98		.00 50.51 B	č
ATOM	6499	CE2 PHE	98		.00 50.40 B	č
ATOM	6500	CZ PHE	98		.00 49.83 B	č
ATOM	6501	C PHE	98		.00 51.24 B	Č
ATOM	6502	0 PHE	98		.00 50.42 B	0
ATOM	6503	N GLY	99	99.770 87.383 47.523 1	.00 50.67 B	N
ATOM	6504	CA GLY	99	98. 383 87. 441 47. 094 1	. 00 48. 74 B	C
ATOM	6505	C GLY	99		.00 47.41 B	C
ATOM	6506	0 GLY	99		. 00 48. 42 B	0
ATOM	6507	N HIS	100		.00 45.49 B	N
ATOM	6508	CA HIS	100		. 00 43. 24 B	C
ATOM	6509	CB HIS	100		.00 41.93 B	C
ATOM	6510	CG HIS	100		.00 39.37 B	C
ATOM	6511	CD2 HIS	100		.00 38.83 B	C
ATOM	6512	NDI HIS	100		.00 39.65 B	N
ATOM ATOM	6513 6514	CE1 HIS NE2 HIS	100		.00 38.90 B	C
ATOM ATOM	6515	C HIS	100 100		.00 38.71 B .00 42.56 B	N C
ATOM	6516	0 HIS	100		.00 42.50 B	0
VIOn	0010	0 1119	100	JJ. JIU 04. 040 41. 413 I	. 00 40. 14 D	U

				14,	FI	G. 4-	134			(Continued)
ATOM	6517	N	SER	101	98. 139	81.547	47.063	1.00 41.90	В	N
ATOM	6518	CA	SER	101	98.716		47.817	1.00 43.20	В	C
ATOM	6519	CB	SER	101	97.623	79. 527	48. 382	1.00 43.41	В	C
ATOM	6520	0G	SER	101	96. 852		47. 354	1.00 44.00	В	0
ATOM	6521	C	SER	101	99. 582		46.820	1.00 42.92	В	C
ATOM	6522	0	SER	101	99.083		45. 794	1.00 43.33	В	0
ATOM	6523	N	ILE	102	100.880		47.095	1.00 41.90	В	Ŋ
ATOM	6524	CA	ILE	102	101.762		46. 183	1.00 42.10	. B	C
ATOM	6525	CB	ILE	102	103. 255		46.369	1.00 43.10	В	C
ATOM	6526		ILE	102	103. 370		46.404	1.00 43.52	В	C
ATOM ATOM	6527 6528		ILE ILE	102 102	103. 824 105. 294		47.660 47.895	1.00 45.01	В	C
ATOM	6529	CDI	ILE	102	103. 294	77. 380	46.415	1.00 46.96 1.00 41.08	B B	C C
ATOM	6530	Õ	ILE	102	101. 677	76. 901	47. 544	1.00 41.03	B B	0
ATOM	6531	Ň	ASN	103	101.342	76.648	45. 339	1.00 41.27	В	N
ATOM	6532	CA	ASN	103	101. 157	75. 211	45. 434	1.00 39.20	В	Č
ATOM	6533	CB	ASN	103	100. 502	74.674	44. 163	1.00 39.98	В	č
ATOM	6534	ČĞ	ASN	103	100. 190		44. 257	1.00 39.82	B	č
ATOM	6535		ASN	103	99.355	72.784	45.056	1.00 40.83	B	Ö
ATOM	6536		ASN	103	100.866	72.396	43.448	1.00 40.75	. B	Ň
ATOM	6537	C	ASN	103	102.486	74.508	45.645	1.00 37.42	В	C
ATOM	6538	0	ASN	103	102.601	73.614	46.475	1.00 38.46	В	0
ATOM	6539	N	ASP	104	103. 491	74.912	44.880	1.00 35.77	В	N
ATOM	6540	CA	ASP	104	104. 808	74.303	44.982	1.00 34.14	В	C
ATOM	6541	CB	ASP	104	104. 819	72.955	44. 248	1.00 33.54	В	C
ATOM	6542	CG	ASP	104	105.987	72.072	44.655	1.00 34.77	В	C
ATOM	6543	OD1		104	106.061	70. 919	44. 178	1.00 33.72	В	0
ATOM	6544	OD2		104	106.835	72. 525	45. 453	1.00 35.84	В	0
ATOM	6545	C	ASP	104	105.827	75. 253	44. 367	1.00 33.07	В	C
ATOM ATOM	6546 6547	O N	ASP TYR	104	105.461	76. 218	43.695	1.00 33.54	В	0
ATOM	6548	CA	TYR	105 105	107. 103 108. 167	74. 985 75. 824	44.607	1.00 32.32	В	N
ATOM	6549	CB	TYR	105	108. 101	76. 573	44. 082 45. 220	1.00 31.45 1.00 32.58	В	C
ATOM	6550	CG	TYR	105	100. 515	75. 662	46. 218	1.00 32.38	B B	C C
ATOM	6551	CD1		105	110. 859	75. 306	46. 091	1.00 36.01	В	C
ATOM	6552	CE1		105	111. 465	74. 453		1.00 36.30	B	C
ATOM	6553	CD2		105	108. 791	75. 138	47. 287	1.00 37.55	B	č
ATOM	6554	CE2		105	109. 387	74. 282	48. 208	1.00 38.47	B	č
ATOM	6555	CZ	TYR	105	110.719	73.947	48.065	1.00 37.17	B	č
ATOM	6556	OH	TYR	105	111. 293	73.106	48.984	1.00 38.67	B	Ö
ATOM	6557		TYR	105	109. 180	74.972	43.347	1.00 30.07	В	Č
ATOM	6558		TYR	105	109.048	73. 754	43. 276	1.00 29.32	В	0
ATOM	6559	N	SER	106	110. 203	75.623	42.815	1.00 28.45	В	N
ATOM	6560		SER	106	111. 236	74. 938	42.059	1.00 26.63	В	C
ATOM	6561	CB	SER	106	110.648	74. 391	40. 758	1.00 24.49	В	С
ATOM	6562		SER	106	111.662	74. 145	39. 806	1.00 24.16	В	0
ATOM	6563		SER	106	112. 341	75. 926	41.745	1.00 26.32	В	C
ATOM ATOM	6564 6565		SER	106	112.168	76. 821	40.919	1.00 28.04	В	0
V I OIM	6565	N	ILE	107	113. 475	75. 770	42.413	1.00 25.01	В	N

										(Continue	ed)
					FIC	G. 4-	1 3 6			,	
ATOM	6615	CZ	PHE	113	117. 386	85. 152	36. 819	1.00 35.71	В	C	
ATOM ATOM	6616 6617	C 0	PHE PHE	113 113	114. 831 115. 308	80. 896 79. 829	41.058 41.425	1.00 30.65 1.00 30.90	B B	C 0	
ATOM	6618	Ň	ILE	114	113.557	81. 205	41.219	1.00 30.09	В	N	
ATOM	6619	CA	ILE	114	112.630	80. 258	41.791	1.00 29.81	В	Č	
ATOM	6620	CB	ILE	114	112. 394	80.504	43. 293	1.00 28.60	В	C	
ATOM	6621		ILE	114	111.911	81.915	43. 529	1.00 29.81	В	C	
ATOM	6622		ILE ILE	114	111.378	79.490	43.813	1.00 30.57 1.00 33.23	В	C C	
ATOM ATOM	6623 6624	CDI	ILE	114 114	111. 336 111. 336	79.367 80.403	45.325 41.019	1.00 33.23	B B	C	
ATOM	6625	Õ	ILE	114	110.895	81.508	40.715	1.00 28.83	В	Ö	
ATOM	6626	Ň	LEU	115	110.756	79. 265	40.671	1.00 30.43	B	Ň	
ATOM	6627	CA	LEU	115	109.516	79. 223	39. 925	1.00 29.05	В	С	
ATOM	6628	CB	LEU	115	109. 596	78. 108	38. 890	1.00 28.31	В	C	
ATOM	6629	CG	LEU	115	108. 449	77. 898	37. 912	1.00 28.22	В	C	
ATOM ATOM	6630 6631		LEU LEU	115 115	108. 425 108. 645	79. 001 76. 553	36. 872 37. 245	1.00 28.47 1.00 29.52	B B	C C	
ATOM	6632	CDZ	LEU	115	108. 043	78. 923	40. 932	1.00 29.52	В	Č	
ATOM	6633	ŏ	LEU	115	108. 370	77. 824	41. 483	1.00 30.72	B	ŏ	
ATOM	6634	Ň	LEU	116	107.568	79.901	41.196	1.00 30.29	B	N	
ATOM	6635	CA	LEU	116	106.479	79.699	42.142	1.00 30.17	В	С	
ATOM	6636	CB	LEU	116	106. 129	81.001	42. 861	1.00 31.28	В	C	
ATOM	6637	CG	LEU	116	107. 277	81.741	43. 544	1.00 33.66	В	C	
ATOM ATOM	6638 6639		LEU LEU	116 116	106. 732 107. 957	82. 988 80. 821	44. 229 44. 552	1.00 33.41 1.00 34.07	B B	C C	
ATOM	6640	C	LEU	116	105. 270	79. 215	41.369	1.00 34.01	В	Č	
ATOM	6641	ŏ	LEU	116	104. 835	79.845	40. 401	1.00 30.69	B	Ŏ	
ATOM	6642	N	GLU	117	104.724	78.091	41.804	1.00 30.37	В	N	
ATOM	6643	CA	GLU	117	103.563	77. 513	41.159	1.00 29.50	В	C	
ATOM	6644	CB	GLU	117	103.813	76.017	40.963	1.00 30.63	В	C	
ATOM ATOM	6645 6646	CG CD	GLU GLU	117	102. 671 103. 023	75. 210 73. 728	40. 368 40. 270	1.00 32.07 1.00 33.58	B B	C C	
ATOM	6647	0E1		117 117	103. 023	73. 341	39. 340	1.00 33.58	В	0	
ATOM	6648		GLU	117	102. 566	72.956	41.140	1.00 32.35	В	Ö	
ATOM	6649	C	GLU	117	102.312	77.756	42.009	1.00 29.67	B	Č	
ATOM	6650	0	GLU	117	102.333	77. 583	43. 228	1.00 27.89	В	0	
ATOM	6651	N	TYR	118	101. 235	78. 184	41.355	1.00 29.27	В	Ŋ	
ATOM	6652	CA	TYR	118	99. 966	78. 423	42.026	1.00 28.00	В	C	
ATOM ATOM	6653 6654	CB CG	TYR TYR	118 118	99. 928 100. 036	79. 818 80. 955	42.643 41.659	1.00 29.37 1.00 29.69	B B	C C	
ATOM	6655		TYR	118	101. 256	81.301	41.092	1.00 20.03	В	Č	
ATOM	6656		TYR	118	101.355	82.373	40. 210	1.00 31.36	B	Č	
ATOM	6657	CD2	TYR	118	98. 915	81.703	41.316	1.00 30.41	В	С	
ATOM	6658		TYR	118	99.003	82. 768	40. 439	1.00 31.17	В	C	
ATOM	6659	CZ	TYR	118	100. 222	83. 101	39. 891	1.00 31.56	В	C	
ATOM	6660 6661	OH C	TYR	118	100. 298	84. 179 78. 240	39. 039 41. 038	1.00 33.43 1.00 27.66	B B	0	
ATOM ATOM	6662	0	TYR TYR	118 118	98. 814 99. 046	78. 240	39. 874	1.00 27.00	B B	C 0	
ATOM	6663	N	ASN	119	97. 582	78. 450	41. 499	1.00 27.22	В	N	
0					21.000			100 51125	_	<u>.</u> .	

ATOM 6664 CA ASN 119 96.397 78.261 40.659 1.00 27.10 B C ATOM 6665 CB ASN 119 96.422 79.203 39.477 1.00 27.52 B C ATOM 6666 CG ASN 119 99.495 80.761 40.456 1.00 26.76 B O ATOM 6667 ODL ASN 119 94.905 80.761 40.456 1.00 26.76 B O ATOM 6668 ND2 ASN 119 96.613 81.612 39.277 1.00 25.87 B N ATOM 6668 ND2 ASN 119 96.613 81.612 39.277 1.00 25.87 B N ATOM 6669 C ASN 119 96.342 76.810 40.171 1.00 27.88 B C ATOM 6670 O ASN 119 96.372 76.534 39.045 1.00 27.93 B O ATOM 6671 N TYR 120 96.771 75.888 41.028 1.00 27.57 B N ATOM 6671 N TYR 120 96.795 74.466 40.702 1.00 29.01 B C ATOM 6673 CB TYR 120 97.396 73.669 41.866 1.00 38.55 B C ATOM 6674 CC TYR 120 97.421 72.171 41.635 1.00 32.83 B C ATOM 6675 CDI TYR 120 98.466 71.568 40.940 1.00 33.76 B C ATOM 6676 CEI TYR 120 98.484 70.190 40.717 1.00 35.03 B C ATOM 6676 CEI TYR 120 99.448 69.403 41.191 1.00 34.35 B C ATOM 6676 CEI TYR 120 97.444 69.403 41.191 1.00 34.35 B C ATOM 6676 CEI TYR 120 97.444 69.403 41.191 1.00 35.03 B C ATOM 6676 CEI TYR 120 97.462 68.039 40.987 1.00 33.76 B C ATOM 6678 CE TYR 120 97.462 68.039 40.987 1.00 33.76 B C ATOM 6680 OH TYR 120 97.462 68.039 40.987 1.00 33.76 B C ATOM 6683 N VAL 121 94.136 72.487 38.842 1.00 1.00 34.41 B C ATOM 6683 N VAL 121 94.336 72.487 38.842 1.00 1.00 35.47 B C ATOM 6683 N VAL 121 94.336 72.487 38.842 1.00 25.45 B C ATOM 6683 C C TYR 120 94.458 74.034 41.099 1.00 35.56 B C ATOM 6683 C C TYR 120 94.458 74.034 41.099 1.00 35.56 B C ATOM 6683 C C TYR 120 94.458 74.034 41.099 1.00 35.56 B C ATOM 6680 C C TYR 120 94.458 74.034 41.099 1.00 35.56 B C ATOM 6680 C C TYR 120 94.458 74.034 41.099 1.00 35.56 B C ATOM 6680 C C TYR 120 94.458 74.034 41.099 1.00 35.56 B C ATOM 6680 C C TYR 120 94.458 74.034 41.099 1.00 35.56 B C ATOM 6680 C C TYR 120 94.558 65.65 B C ATOM 6680 C C TYR 120 94.558 65.65 B C ATOM 6680 C C TYR 120 94.458 74.034 1.00 21.01 B C ATOM 6690 N L TYS 122 94.66 68.73 31.483 39.248 1.00 21.18 B C ATOM 6690 N L TYS 122 94.66 68.73 31.483 39.248 1.00 22.12 B C ATOM 6690 N L TYS 122 94.66 68.73 31.483 39.248 1.00 20.04 B C											(Continued)
ATOM 6665 CB ASN 119 95.918 80.599 39.777 1.00 27.22 B C ATOM 6666 CG ASN 119 95.918 80.599 39.777 1.00 27.62 B C ATOM 6667 ODI ASN 119 94.905 80.761 40.456 1.00 26.76 B O ATOM 6668 ND2 ASN 119 94.613 81.612 39.277 1.00 25.87 B N ATOM 6669 C ASN 119 95.613 81.612 39.277 1.00 27.88 B C ATOM 6670 O ASN 119 95.923 76.534 39.045 1.00 27.93 B O ATOM 6671 N TYR 120 96.771 75.888 41.028 1.00 27.57 B N ATOM 6671 N TYR 120 96.771 75.888 41.028 1.00 27.57 B N ATOM 6672 CA TYR 120 95.795 74.466 40.702 1.00 29.01 B C ATOM 6673 CB TYR 120 97.421 72.171 41.635 1.00 23.83 B C ATOM 6676 CD TYR 120 97.421 72.171 41.635 1.00 23.83 B C ATOM 6676 CD TYR 120 98.466 71.568 40.940 1.00 33.76 B C ATOM 6676 CD TYR 120 98.484 70.190 40.717 1.00 35.03 B C ATOM 6676 CD TYR 120 98.484 70.190 40.717 1.00 35.03 B C ATOM 6676 CD TYR 120 98.484 70.190 40.717 1.00 35.03 B C ATOM 6677 CD TYR 120 97.444 69.403 41.191 1.00 34.31 B C ATOM 6677 CD TYR 120 97.446 69.403 41.191 1.00 34.35 B C ATOM 6681 C TYR 120 97.446 69.403 41.191 1.00 35.47 B C ATOM 6681 C TYR 120 97.446 69.403 41.191 1.00 35.47 B C ATOM 6681 C TYR 120 97.446 69.403 41.191 1.00 35.47 B C ATOM 6681 C TYR 120 97.446 69.403 41.191 1.00 35.47 B C ATOM 6688 CD ATOM 6681 C TYR 120 97.446 69.403 41.191 1.00 35.47 B C ATOM 6688 CD ATOM 6689 CD ATOM 6						FIG.	4 -	1 3 7			(Continued)
ATOM 6665 CB ASN 119 95.422 79.203 39.449 1.00 27.22 B C ATOM 6666 CG ASN 119 95.918 80.599 39.777 1.00 27.62 B C ATOM 6668 ND2 ASN 119 94.905 80.761 40.456 1.00 26.76 B O ATOM 6668 ND2 ASN 119 94.613 81.612 39.277 1.00 27.88 B C ATOM 6669 C ASN 119 95.618 80.541 76.810 40.171 1.00 27.88 B C ATOM 6670 O ASN 119 95.923 76.534 39.045 1.00 27.93 B O ATOM 6671 N TYR 120 96.795 74.466 40.702 1.00 29.01 B C ATOM 6672 CA TYR 120 96.795 74.466 40.702 1.00 29.01 B C ATOM 6673 CB TYR 120 97.421 72.171 41.635 1.00 27.57 B N ATOM 6673 CB TYR 120 97.421 72.171 41.635 1.00 33.85 B C ATOM 6675 CD1 TYR 120 98.466 71.568 40.940 1.00 33.76 B C ATOM 6676 CE TYR 120 98.484 70.190 40.717 1.00 35.03 B C ATOM 6676 CE TYR 120 98.484 70.190 40.717 1.00 35.03 B C ATOM 6677 CD2 TYR 120 98.484 70.190 40.717 1.00 35.03 B C ATOM 6677 CD2 TYR 120 97.444 69.403 41.191 1.00 34.35 B C ATOM 6677 CT TYR 120 97.446 69.403 41.191 1.00 34.35 B C ATOM 6688 CD TYR 120 94.458 74.034 41.880 1.00 34.35 B C ATOM 6688 CD TYR 120 94.458 74.034 41.890 1.00 35.56 B C ATOM 6688 CD TYR 120 95.438 74.034 41.099 1.00 35.56 B C ATOM 6688 CD TYR 120 94.458 74.034 41.099 1.00 35.56 B C ATOM 6688 CD TYR 120 94.458 74.034 41.099 1.00 35.56 B C ATOM 6688 CD TYR 120 94.458 74.034 41.099 1.00 35.56 B C ATOM 6688 CD TYR 120 94.458 74.034 41.099 1.00 31.09 B O ATOM 6684 CA VAL 121 94.136 72.427 38.842 1.00 27.53 B N ATOM 6684 CA VAL 121 94.36 72.427 38.842 1.00 27.53 B N ATOM 6689 CD TYR 120 94.458 74.034 41.099 1.00 31.09 B C ATOM 6689 CD TYR 120 94.458 74.034 41.099 1.00 32.55 B C ATOM 6689 CD TYR 120 94.458 74.034 41.099 1.00 31.09 B C ATOM 6689 CD TYR 120 94.458 74.034 41.00 22.15 B C ATOM 6689 CD TYR 120 94.458 74.034 41.00 22.15 B C ATOM 6689 CD TYR 120 94.458 74.034 41.00 22.18 B C ATOM 6690 N LYS 122 94.506 68.808 37.18 39.00 1.00 24.18 B C ATOM 6690 N LYS 122 94.456 68.609 39.77 1.00 23.23 B C ATOM 6690 N LYS 122 94.456 68.609 39.77 1.00 23.23 B C ATOM 6697 C LYS 122 94.506 66.433 32.948 1.00 23.23 B C ATOM 6697 C LYS 122 94.406 68.609 37.57 1.00 24.10 B C ATOM 67	ATOM	6664	CA	ASN	119	96. 397	78. 261	40.659	1.00 27.10	В	С
ATOM 6668 ND2 ASN 119 94.905 80.761 40.456 1.00 26.76 B O ATOM 66689 C ASN 119 96.613 81.612 39.277 1.00 25.87 B N ATOM 6670 O ASN 119 95.923 76.534 39.045 1.00 27.93 B O ATOM 6671 N TYR 120 96.795 74.466 40.702 1.00 29.01 B C ATOM 6672 CA TYR 120 97.496 73.669 41.866 1.00 30.85 B C ATOM 6673 CB TYR 120 97.421 72.171 41.635 1.00 27.57 B N ATOM 6676 CD I TYR 120 97.421 72.171 41.635 1.00 23.83 B C ATOM 6676 CD I TYR 120 98.466 71.568 40.940 1.00 33.76 B C ATOM 6677 CD TYR 120 98.466 71.568 40.940 1.00 33.76 B C ATOM 6677 CD TYR 120 98.484 70.190 40.717 1.00 33.76 B C ATOM 6677 CD TYR 120 98.484 70.190 40.717 1.00 33.76 B C ATOM 6677 CD TYR 120 97.444 69.403 41.191 1.00 34.35 B C ATOM 6679 CZ TYR 120 97.444 69.403 41.191 1.00 35.47 B C ATOM 6678 CZ TYR 120 97.446 68.039 40.987 1.00 34.35 B C ATOM 6680 CH TYR 120 97.446 68.039 40.987 1.00 35.56 B C ATOM 6680 CH TYR 120 97.446 68.039 40.987 1.00 35.56 B C ATOM 6680 CH TYR 120 97.445 68.039 40.987 1.00 35.56 B C ATOM 6687 CZ TYR 120 97.445 68.039 40.987 1.00 35.56 B C ATOM 6687 CZ TYR 120 97.445 68.039 40.987 1.00 35.56 B C ATOM 6687 CZ TYR 120 97.445 68.039 40.987 1.00 35.56 B C ATOM 6687 CZ TYR 120 97.445 68.039 40.987 1.00 35.56 B C ATOM 6687 CZ TYR 120 97.445 68.039 40.987 1.00 35.56 B C ATOM 6687 CZ TYR 120 94.458 74.034 41.099 1.00 31.09 B O ATOM 6688 C C TYR 120 94.458 74.034 41.092 1.00 25.45 B C ATOM 6687 CZ TYR 120 94.458 74.034 41.092 1.00 25.45 B C ATOM 6687 CZ TYR 120 94.458 74.034 41.092 1.00 25.45 B C ATOM 6688 C C TYR 121 94.136 72.487 38.842 1.00 27.53 B N ATOM 6688 C C TYR 121 94.458 74.034 41.092 1.00 23.18 B C ATOM 6689 C C TYR 121 94.458 74.034 41.092 1.00 23.05 B C ATOM 6690 C TYR 122 94.458 74.034 41.092 1.81 B C ATOM 6690 C TYR 122 94.458 68.83 71.33 8.7376 1.00 24.18 B C ATOM 6690 C TYR 122 94.466 68.35 38.971 1.00 24.18 B C ATOM 6690 C TYR 122 94.466 68.373 38.970 1.00 24.18 B C ATOM 6690 C TYR 122 94.466 68.66 63.37 39.390 1.00 20.04 B C ATOM 6690 C TYR 122 94.406 66.395 04.0161 1.00 20.35 B C ATOM 6690 C TYR 122 94.506 66.66 31.37 37.87 1	ATOM		CB	ASN	119						
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ATOM	6713	CE2 T	'RP	124	92. 630	63. 449	31.455	1.00 16.84	В	С
ATOM	6714	CE3 T		124	91.909	62.942	33.713	1.00 17.02	В	C
ATOM	6715	CD1 T	rp	124	94.819	62.999	31.539	1.00 19.00	В	С
ATOM	6716	NE1 T		124	93. 794	63.429	30.731	1.00 18.26	В	N
ATOM	6717	CZ2 I	TRP	124	91.331	63.815	31.067	1.00 15.16	В	C
ATOM	6718	CZ3 1		124	90.615	63.305	33. 326	1.00 16.85	В	С
ATOM	6719	CH2 T		124	90. 342	63. 737	32.011	1.00 16.12	В	C
ATOM	6720		rp -	124	95.718	62.679	36. 427	1.00 17.28	В	C
ATOM	6721		CRP	124	95.816	63. 437	37. 397	1.00 17.74	В	0
ATOM	6722		ARG	125	96.430	61.560	36. 339	1.00 15.31	В	N
ATOM	6723		ARG	125	97.317	61.185	37. 429	1.00 16.66	В	C
ATOM	6724		ARG	125	97.666	59. 702	37. 323	1.00 16.96	В	C
ATOM	6725		ARG	125	98. 908	59. 288	38.076	1.00 18.35	В	C
ATOM	6726		ARG	125	98.689	57. 987	38. 794	1.00 18.85	В	C
ATOM	6727		ARG	125	98. 049	56.965	37. 972	1.00 18.57	В	N C
ATOM	6728		ARG	125	97. 547	55.842	38. 475	1.00 17.58	В	C
MOTA	6729	NH1 A		125	96. 972 97. 626	54. 944 55. 621	37. 693 39. 776	1.00 16.96 1.00 17.03	B B	N N
MOTA	6730 6731	NH2 A	ang ARG	125 125	98. 582	62. 027	37. 568	1.00 11.03	В	C
ATOM ATOM	6732		ang ARG	125	99. 075	62. 227	38. 674	1.00 18.04	В	0
ATOM	6733		HIS	126	99. 099	62. 533	36. 454	1.00 10.00	В	N
ATOM	6734		HS	126	100. 300	63. 353	36. 487	1.00 18.20	В	Č
ATOM	6735		HIS	126	101.391	62.673	35. 673	1.00 18.72	В	č
ATOM	6736		HIS	126	101.721	61. 295	36. 151	1.00 19.88	В	č
ATOM	6737	CD2 F		126	101.519	60.084	35. 581	1.00 20.06	B	č
ATOM	6738	ND1 H		126	102. 341	61.054	37. 360	1.00 17.75	B	· N
ATOM	6739	CE1 I		126	102.510	59. 753	37. 512	1.00 19.55	B	Ċ
ATOM	6740	NE2 I		126	102.019	59.142	36.447	1.00 22.65	В	N
ATOM	6741		HIS	126	100.079	64.772	35.966	1.00 18.28	В	C
ATOM	6742		RIF	126	100.692	65.716	36, 462	1.00 18.27	В	0
ATOM	6743	N S	SER	127	99. 204	64. 921	34.974	1.00 16.08	В	N
ATOM	6744		SER	127	98. 936	66.230	34. 382	1.00-16.78	В	С
ATOM	6745		SER	127	98. 209	66.070	33. 037	1.00 15.96	В	C
ATOM	6746		SER	127	96.999	65. 349	33. 179	1.00 17.80	В	0
ATOM	6747		SER	127	98. 151	67. 203	35. 261	1.00 16.75	В	С
ATOM	6748		SER	127	97. 523	66.816	36. 247	1.00 17.88	В	0
ATOM	6749		ryr	128	98. 205	68. 473	34. 873	1.00 15.65	В	N
ATOM	6750		ryr	128	97. 520	69. 556	35. 559	1.00 17.91	В	Ċ
ATOM	6751		ryr	128	97. 815	69. 506	37.060	1.00 17.70	В	C
ATOM	6752		ryr	128	99. 253	69. 796	37. 444	1.00 17.20	В	C
ATOM	6753		ryr	128	99. 725	71.107	37. 540	1.00 16.17	В	C
ATOM	6754	CE1 7	LXK	128	101.036	71.375	37. 927	1.00 16.04	В	C
ATOM	6755	CD2		128	100. 135	68.759	37. 739	1.00 17.12	В	C
ATOM	6756 6757	CE2 7		128	101.449	69.016	38. 123	1.00 15.90	В	C
MOTA	6757 6758		ryr ryd	128	101.891	70.322	38. 216	1.00 17.19 1.00 20.16	B	C
MOTA	6758 6750		FYR FVD	128	103. 190	70. 572 70. 897	38. 603 34. 992	1.00 20.16	B B	0 C
ATOM	6759 6760		FYR FYR	128 128	97. 977	70. 897	34. 268	1.00 19.77	В	0
ATOM ATOM	6761		i i k CHR	128	98. 970	71.955	34. 208 35. 291	1.00 21.70	В	N N
ATOM	0101	ix]	ш	149	97. 239	(1.500	00.471	1.00 60.40	D	IX

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ATOM	6762	CA	THR	129	97. 647	73. 276	1 3 9 34.840	1.00 22.26	В	С
ATOM	6763	CB	THR	129	96. 599	73. 968	33. 950	1.00 23.04	В	č
ATOM	6764		THR	129	95. 353	74. 045	34. 652	1.00 24.93	В	ŏ
ATOM	6765		THR	129	96. 428	73. 213	32. 634	1.00 22.70	B	Č
ATOM	6766	C	THR	129	97. 856	74. 136	36.069	1.00 22.23	B	Č
ATOM	6767	Ö	THR	129	97.462	73. 765	37. 182	1.00 20.98	B	0
ATOM	6768	N	ALA	130	98. 474	75. 289	35.854	1.00 22.77	В	N
ATOM	6769	CA	ALA	130	98. 754	76. 222	36.926	1.00 23.41	B .	C
ATOM	6770	CB	ALA	130	99. 789	75. 631	37.859	1.00 19.73	В	C
ATOM	6771	C	ALA	130	99.269	77. 525	36. 338	1.00 26.66	В	C
ATOM	6772	0	ALA	130	99. 514	77. 632	35. 133	1.00 27.20	В	0
ATOM	6773	N	SER	131	99. 414	78. 523	37. 199	1.00 29.67	В	N
ATOM	6774	CA	SER	131	99. 934	79. 818	36. 796	1.00 30.14	В	C
ATOM	6775	CB	SER	131	99.056	80. 948	37. 333	1.00 30.56	В	C
ATOM	6776	0G	SER	131	97. 713	80. 775	36. 913	1.00 32.67	В	0
ATOM	6777	C	SER	131	101. 290	79.851	37. 463	1.00 31.00	В	C
ATOM	6778	0	SER	131	101.448	79. 334	38. 569	1.00 30.79	В	0
ATOM	6779	N	TYR	132	102. 272	80. 438	36. 792	1.00 32.02	В	N
ATOM	6780	CA	TYR	132	103.611	80. 506	37. 347	1.00 31.40	В	C
ATOM ATOM	6781 6782	CB CG	TYR TYR	$\begin{array}{c} 132 \\ 132 \end{array}$	104. 558	79.634	36.519	1.00 28.72	В	C
ATOM	6783		TYR	132	104. 179 103. 082	78. 174 77. 721	36. 516 35. 791	1.00 26.74 1.00 26.31	В	C
ATOM	6784		TYR	132	103. 082	76. 383	35. 834	1.00 26.31	B B	C C
ATOM	6785		TYR	132	102.030	77. 250	37. 283	1.00 26.45	В	Č
ATOM	6786		TYR	132	104. 510	75. 911	37. 332	1.00 20.38	В	C
ATOM	6787	CZ	TYR		103. 415	75. 486	36. 609	1.00 25.59	В	C
ATOM	6788	OH	TYR	132	103. 023	74. 171	36. 677	1.00 25.63	В	Õ
ATOM	6789	C	TYR	132	104. 143	81. 929	37.411	1.00 32.91	В	č
ATOM	6790	ŏ	TYR	132	103. 743	82. 790	36. 636	1.00 34.01	В	ŏ
ATOM	6791	N	ASP	133	105. 041	82. 165	38. 358	1.00 35.11	B	Ň
ATOM	6792	CA	ASP	133	105.674	83.465	38. 539	1.00 36.35	B	Ċ
ATOM	6793	CB	ASP	133	104. 954	84. 287	39.614	1.00 38.51	B	č
ATOM	6794	CG	ASP	133	103.732	85.008	39.074	1.00 41.22	B	Č
ATOM	6795	OD1	ASP	133	102.805	84. 332	38.580	1.00 42.20	В	0
ATOM	6796	0D2	ASP	133	103.702	86. 253	39.139	1.00 42.84	В	0
ATOM	6797	C	ASP	133	107.112	83. 228	38.954	1.00 35.61	В	C
ATOM	6798	0	ASP	133	107. 385	82.438	39.855	1.00 35.76	В	0
ATOM	6799	N	ILE	134	108. 031	83. 908	38. 285	1.00 35.21	В	N
ATOM	6800	CA	ILE	134	109. 444	83. 764	38. 585	1.00 34.01	В	С
ATOM	6801	CB	ILE	134	110. 267	83. 750	37. 287	1.00 33.62	В	C
ATOM	6802	CG2		134	111.718	83. 392	37. 593	1.00 31.90	В	С
ATOM	6803	CG1		134		82. 737	36. 312	1.00 32.72	В	Č
ATOM	6804	CD1		134		82. 794	34. 909	1.00 31.29	В	C
ATOM	6805	C	ILE	134	109. 887	84. 911	39. 483	1.00 34.02	В	C
ATOM	6806	0 N	ILE	134	109. 521	86.065	39. 261	1.00 33.25	В	0
ATOM	6807 6808	N	TYR	135	110.662	84. 573	40.507	1.00 35.09	В	N
ATOM ATOM	6809		TYR TYR	135 135	111. 167	85. 539	41.475	1.00 36.09	В	C
ATOM	6810		TYR	135		85. 174	42.868	1.00 36.02 1.00 36.66	B B	C C
WIOM	0010	U	111	100	111. 222	86.011	44.000	1.00 90.00	В	C

					٠.				(Continued)
					FIG.	4 - 14()		(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6811 6812 6813 6814 6815 6816 6817 6818 6820 6821 6822 6823 6824 6825 6826 6827 6828 6829 6830 6831 6832	CZ OH C O N CA CB CG OD1 OD2 C O CA CB CG CD1 CD2	TYR TYR TYR TYR TYR TYR TYR ASP ASP ASP ASP ASP ASP LEU LEU LEU LEU LEU LEU	135 135 135 135 135 135 136 136 136 136 136 136 137 137	110. 635 87 111. 134 87 112. 332 85 112. 839 86 112. 235 87 112. 740 88 112. 688 85 113. 293 84 113. 304 86 114. 759 86 115. 187 87 116. 690 88 117. 107 88 117. 456 87 115. 316 86 114. 972 87 116. 181 85 116. 761 85 117. 219 84 116. 058 83 116. 582 81 115. 199 83	4 - 1 4 (. 222	3 1.00 34.73 4 1.00 35.12 5 1.00 35.07 1 1.00 35.31 9 1.00 35.05 0 1.00 38.19 3 1.00 37.81 4 1.00 40.56 5 1.00 42.09 7 1.00 42.45 1.00 43.61 8 1.00 45.53 1 1.00 41.77 1 1.00 42.49 6 1.00 42.49 1 1.00 42.49 1 1.00 48.88 7 1.00 48.88 7 1.00 48.91	B B B B B B B B B B B B B B B B B B B	(Continued) C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6830 6831 6832 6833 6834 6835 6836 6837 6840 6841 6842 6843 6844 6845 6846 6847 6848 6849 6850 6851	CG CD1 CD2 C O N CA CB CG OD1 ND2 C O CA CB CC CD CC CD CC O CC O CC O CC O CC O	LEU LEU LEU LEU ASN ASN ASN ASN ASN ASN LYS LYS LYS LYS LYS LYS LYS LYS	137 137 137 137 138 138 138 138 138 138 138 139 139 139 139 139 139 139	116. 058 83 116. 582 81 115. 199 83 117. 908 86 118. 309 86 118. 429 87 119. 522 88 120. 330 88 120. 728 86 121. 232 85 120. 512 86 118. 935 89 119. 259 90 118. 064 89 117. 417 91 116. 807 91 117. 726 91 116. 996 91 117. 887 91 116. 302 91 116. 302 91 115. 669 92	136 44.11 716 43.99 291 45.36 544 44.22 750 45.37 139 43.16 3.151 41.98 5.530 40.19 472 43.56 101 44.57 228 42.24 5.530 40.19 42.28 42.24 5.530 40.19 42.28 42.24 5.520 40.29 8.657 41.48 520 40.29 874 39.00 650 37.79 183 43.85 202 44.13	7 1.00 49.07 1 1.00 50.17 1 1.00 48.91 8 1.00 50.19 0 1.00 51.45 0 1.00 52.26 0 1.00 53.21 3 1.00 54.36 4 1.00 56.39 4 1.00 56.67 7 1.00 54.11 1 1.00 54.39 1 1.00 55.06 4 1.00 55.06 1 1.00 56.75 0 1.00 58.34 1 1.00 59.63 3 1.00 61.32 8 1.00 62.59 7 1.00 56.78 9 1.00 57.22	B B B B B B B B B B B B B B B B B B B	C C C C O N C C C O N C C C C C N C O
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6852 6853 6854 6855 6856 6857 6858 6859	N CA CB CG CD NE CZ NH1	ARG ARG ARG ARG ARG ARG ARG	140 140 140 140 140 140 140 140	114. 994 89 115. 433 90 116. 063 89 116. 091 89 116. 578 88 115. 979 87	0.006 44.42 0.838 45.40 0.341 46.78 0.260 47.64 0.658 49.11 3.575 49.97 7.394 50.11 7.124 49.45	9 1.00 57.44 7 1.00 58.40 9 1.00 61.65 6 1.00 64.17 2 1.00 67.20 2 1.00 68.02	B B B B B	N C C C C N C N

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		FIG. 4-141	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6861	140	B O N C C C C C C C C C C C C C C C C C C

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					(Continued)
				FIG. 4-143	, • • • • • • • • • • • • • • • • • • •
ATOM ATOM ATOM ATOM ATOM	6958 6959 6960 6961 6962	OG1 THR CG2 THR C THR O THR N GLN	152 152 152 152 153	102. 882 76. 231 31. 643 1. 00 24. 98 100. 257 75. 012 31. 791 1. 00 22. 65 99. 908 74. 652 32. 912 1. 00 21. 72	B
ATOM ATOM ATOM	6963 6964 6965	CA GLN CB GLN CG GLN	153 153 153	100. 407 72. 730 31. 010 1. 00 20. 14 100. 023 72. 081 29. 691 1. 00 20. 22	B C B C
ATOM ATOM ATOM ATOM	6966 6967 6968 6969	CD GLN OE1 GLN NE2 GLN C GLN	153 153 153 153	99. 365 73. 054 26. 939 1. 00 24. 47 97. 600 71. 703 27. 200 1. 00 20. 51	B C B O B N B C
ATOM ATOM ATOM	6970 6971 6972	0 GLN N TRP CA TRP	153 154 154	101.574 70.996 32.154 1.00 22.44 102.794 72.729 31.422 1.00 20.43 104.043 72.189 31.934 1.00 18.53	B O B N B C
ATOM ATOM ATOM ATOM	6973 6974 6975 6976	CB TRP CG TRP CD2 TRP CE2 TRP	154 154 154 154	105. 678 70. 257 31. 719 1. 00 19. 59 105. 891 69. 559 32. 955 1. 00 17. 98	B C B C B C
ATOM ATOM ATOM ATOM	6977 6978 6979 6980	CE3 TRP CD1 TRP NE1 TRP CZ2 TRP	154 154 154 154	105. 058 69. 184 34. 015 1. 00 16. 08 106. 893 70. 316 31. 101 1. 00 20. 53 107. 849 69. 705 31. 877 1. 00 22. 41	B C B C B N
ATOM ATOM ATOM	6981 6982 6983	CZ3 TRP CH2 TRP C TRP	154 154 154	105. 614 68. 502 35. 097 1. 00 14. 46 106. 981 68. 191 35. 130 1. 00 14. 70 105. 172 73. 186 31. 757 1. 00 18. 38	B C B C B C B C
ATOM ATOM ATOM ATOM	6984 6985 6986 6987	O TRP N VAL CA VAL CB VAL	154 155 155 155	106. 139 73. 118 32. 658 1. 00 18. 34 107. 280 74. 010 32. 627 1. 00 20. 45	B O B N B C B C
ATOM ATOM ATOM ATOM	6988 6989 6990 6991	CG1 VAL CG2 VAL C VAL O VAL	155 155 155 155	106. 881 74. 954 34. 937 1. 00 21. 60 108. 180 76. 281 33. 260 1. 00 20. 89 108. 439 73. 255 33. 236 1. 00 21. 60	B C B C B C
ATOM ATOM ATOM	6992 6993 6994	N THR CA THR CB THR	156 156 156	109.647 73.590 32.806 1.00 22.32 110.826 72.929 33.325 1.00 23.44 111.028 71.569 32.677 1.00 24.53	
ATOM ATOM ATOM ATOM	6995 6996 6997 6998	OG1 THR CG2 THR C THR O THR	156 156 156 156	112.350 71.113 32.972 1.00 25.64 H 110.856 71.662 31.166 1.00 25.95 H 112.092 73.727 33.094 1.00 24.37 H 112.305 74.274 32.010 1.00 25.56	3 C 3 C
ATOM ATOM ATOM ATOM	6999 7000 7001 7002	N TRP CA TRP CB TRP CG TRP	157 157 157	112. 929 73. 795 34. 123 1. 00 23. 78 114. 192 74. 500 34. 021 1. 00 22. 95 114. 848 74. 650 35. 399 1. 00 22. 02	B N B C B C
ATOM ATOM ATOM	7003 7004 7005	CD2 TRP CE2 TRP CE3 TRP	157 157 157 157	114. 239 75. 678 36. 293 1. 00 21. 39 E 114. 197 77. 091 36. 070 1. 00 22. 25 E 113. 533 77. 668 37. 177 1. 00 23. 29 E 114. 658 77. 928 35. 046 1. 00 21. 12	B C
ATOM	7006	CD1 TRP	157	113.621 75.460 37.492 1.00 22.04 B	

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					(Continued)
				FIG. 4-144	
ATOM ATOM ATOM	7007 7008 7009	NE1 TRP CZ2 TRP CZ3 TRP	157 157 157	113. 193 76. 650 38. 030 1. 00 22. 01 113. 317 79. 051 37. 286 1. 00 22. 77 114. 445 79. 299 35. 156 1. 00 22. 58	B N B C B C
ATOM	7010	CH2 TRP	157	113.779 79.846 36.270 1.00 21.74	в с
ATOM ATOM	7011 7012	C TRP O TRP	157 157	115. 096 73. 640 33. 153 1. 00 22. 79 114. 789 72. 483 32. 882 1. 00 23. 16	B C B 0
ATOM ATOM	7013 7014	N SER CA SER	158 158	116. 198 74. 211 32. 697 1. 00 21. 93 117. 154 73. 441 31. 928 1. 00 22. 68	B N B C
ATOM	7015	CB SER	158	118.104 74.377 31.172 1.00 23.20	В С
ATOM ATOM	7016 7017	OG SER C SER	158 158	118.550 75.444 31.996 1.00 22.94 117.898 72.667 33.017 1.00 23.12	B 0 B C
ATOM	7018	O SER	158	117. 800 73. 006 34. 198 1. 00 23. 58	. B 0
ATOM ATOM	7019 7020	N PRO CD PRO	159 159	118. 641 71. 619 32. 650 1. 00 23. 10 118. 927 71. 096 31. 307 1. 00 23. 69	B N B C
ATOM	7021	CA PRO	159	119. 362 70. 860 33. 679 1. 00 24. 10	B C
ATOM ATOM	7022 7023	CB PRO CG PRO	159 159	120. 041 69. 744 32. 886 1. 00 24. 45 119. 230 69. 660 31. 599 1. 00 23. 97	B C B C
ATOM	7024	C PRO	159	120. 384 71. 738 34. 391 1. 00 25. 41	B C
ATOM ATOM	7025 7026	O PRO N VAL	159 160	120. 598 71. 619 35. 589 1. 00 26. 39 121. 014 72. 619 33. 627 1. 00 27. 71	B O B N
ATOM	7027	CA VAL	160	122.031 73.517 34.146 1.00 29.28	B C
ATOM ATOM	7028 7029	CB VAL CG1 VAL	160 160	123. 383 73. 272 33. 438 1. 00 30. 65 124. 421 74. 249 33. 939 1. 00 33. 70	B C B C
ATOM	7030	CG2 VAL	160	123.844 71.840 33.670 1.00 31.96	B C
ATOM ATOM	7031 7032	C VAL O VAL	160 160	121.606 74.952 33.885 1.00 29.74 120.889 75.224 32.923 1.00 30.93	B C B O
ATOM	7033	N GLY	161	122.043 75.866 34.745 1.00 29.32	B N
ATOM ATOM	7034 7035	CA GLY C GLY	161 161	121.706 77.266 34.562 1.00 28.43 120.289 77.645 34.944 1.00 28.19	B C B C
ATOM	7036	O GLY	161	119.839 77.359 36.053 1.00 30.02	B 0
ATOM ATOM	7037 7038	N HIS CA HIS	162 162	119. 584 78. 296 34. 025 1. 00 26. 53 118. 222 78. 721 34. 290 1. 00 25. 12	B N B C
ATOM	7039	CB HIS	162	118. 214 79. 959 35. 177 1. 00 26. 70	B C
ATOM ATOM	7040 7041	CG HIS	162 162	119.019 81.094 34.629 1.00 29.24 118.664 82.148 33.857 1.00 30.20	B C B C
ATOM	7042	ND1 HIS	162	120. 378 81. 208 34. 830 1. 00 29. 95	B N
ATOM ATOM	7043 7044	CE1 HIS NE2 HIS	162 162	120. 824 82. 283 34. 207 1. 00 30. 75 119. 804 82. 871 33. 608 1. 00 30. 77	B C B N
ATOM	7045	C HIS	162	117. 384 79. 021 33. 059 1. 00 24. 68	. В С
ATOM ATOM	7046 7047	O HIS . N LYS	162 163	116. 730 80. 061 33. 007 1. 00 24. 17 117. 406 78. 135 32. 067 1. 00 22. 79	B O B N
ATOM	7048	CA LYS	163	116. 575 78. 340 30. 889 1. 00 23. 10	B C
ATOM ATOM	7049 7050	CB LYS	163 163	117. 113 77. 578 29. 675 1. 00 22. 90 118. 367 78. 184 29. 063 1. 00 23. 40	B C B C
ATOM	7051	CD LYS	163	118. 797 77. 407 27. 841 1. 00 22. 69	B C
ATOM ATOM	7052 7053	CE LYS NZ LYS	163 163	120. 103 77. 930 27. 282 1. 00 23. 67 120. 616 77. 045 26. 195 1. 00 24. 56	B C B N
ATOM	7054	C LYS	163	115. 215 77. 779 31. 266 1. 00 24. 15	B C
ATOM	7055	O LYS	163	115. 079 77. 104 32. 282 1. 00 24. 69	B 0

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									(Continue	ed)
				FIC	G. 4-	146				
ATOM	7105	CG AS	SN 169	96. 682	77.615	24.662	1.00 27.95	В	С	
ATOM	7106	OD1 AS		96. 240	78.640	24. 150	1.00 32.66	B	0	
ATOM	7107	ND2 AS		96.570		25.961	1.00 30.33	В	N	
ATOM	7108		SN 169	98.463		23.655	1.00 21.23	В	С	
ATOM	7109		SN 169	98. 455	74. 541	22.441	1.00 22.01	В	0	
ATOM	7110		SN 170	99. 031	73. 283	24. 221	1.00 20.60	В	N	
ATOM	7111		SN 170	99.661	72. 208	23.459	1.00 20.97	В	C	
ATOM	7112		SN 170	98. 615	71.515	22.592	1.00 18.68	В	C	
ATOM	7113	CG AS	SN 170	97.629	70. 741	23.412	1.00 18.15	В	C	
ATOM	7114	OD1 AS		97. 158		24.440	1.00 16.27	В	0	
ATOM	7115	ND2 AS		97. 300		22.966	1.00 18.92	В	N	
ATOM	7116		SN 170	100.859		22.598	1.00 21.31	В	Ç	
ATOM	7117		SN 170	101.194		21.659	1.00 20.36	В	0	
ATOM	7118		SP 171	101. 504		22.916	1.00 22.16	В	N	
ATOM	7119	CA AS		102.671	74. 122	22. 160	1.00 23.35	В	C	
ATOM	7120		SP 171	102. 354		21.334	1.00 23.05	В	C	
ATOM	7121	CG AS		101.794		19.978	1.00 23.72	В	C	
ATOM	7122	OD1 AS		102.505	74. 338	19. 210	1.00 23.33	В	0	
ATOM	7123	OD2 AS		100.650		19.679 23.073	1.00 26.97 1.00 23.59	В	0	
ATOM	7124	C AS		103.850		24. 264	1.00 23.39	В	C 0	
ATOM ATOM	7125 7126	0 AS	SP 171 LE 172	103. 672 105. 051	74. 647 74. 301	24. 204 22. 508	1.00 24.16	B B	N N	
ATOM	7127		LE 172	106. 273	74. 497	23. 281	1.00 25.00	В	C	
ATOM	7128		LE 172	107. 353	73. 456	22. 885	1.00 23.23	. В	C	
ATOM	7129	CG2 II		108. 480		23. 896	1.00 23.11	. В В	Č	
ATOM	7130	CG1 II		106. 743	72.056	22. 846	1.00 23.95	В	Č	
ATOM	7131	CD1 II		107. 707	70.986	22. 374	1.00 23.66	В	Č	
ATOM	7132		LE 172	106. 878	75. 892	23. 129	1.00 25.59	B	Č	
ATOM	7133		LE 172	106. 881	76.474	22.048	1.00 25.83	B	0	
ATOM	7134		YR 173	107. 389	76.414	24. 236	1.00 26.85	В	N	
ATOM	7135		YR 173	108.025	77.720	24.272	1.00 27.95	В	C	
ATOM	7136	CB T	YR 173	107.111	78.760	24.933	1.00 27.81	В	С	
ATOM	7137	CG T	YR 173	105.822	79.002	24.190	1.00 29.53	В	С	
ATOM	7138	CD1 T		104. 788	78.063	24. 226	1.00 29.72	В	C	
ATOM	7139		YR 173	103. 599	78. 271	23. 535	1.00 29.08	В	C	
ATOM	7140	CD2 T		105. 634	80. 162		1.00 28.71	В	C	
ATOM	7141	CE2 T		104. 444	80. 381	22. 740	1.00 30.14	В	C	
ATOM	7142		YR 173	103. 432	79. 429	22. 794	1.00 30.82	В	C	
ATOM	7143		YR 173	102. 258		22. 103	1.00 31.14	В	0	
ATOM	7144		YR 173	109. 308	77. 592	25. 080	1.00 28.66	В	C	
ATOM	7145		YR 173	109. 412	76. 735	25. 960	1.00 28.10	В	0	
ATOM	7146	N V		110. 276	78. 451	24. 782	1.00 29.35	В	N	
ATOM	7147	CA V		111.551	78.443	25. 480	1.00 29.22 1.00 29.66	В	C	
ATOM	7148	CB V		112.669	77.855	24. 587	1.00 29.00	B B	C	
ATOM	7149 7150	CG1 V/		114.006	77. 936 76. 403	25. 303 24. 231	1.00 30.07	В	C C	
ATOM ATOM	7150	C V		112. 351 111. 953	70. 403 79. 857	24. 231 25. 887	1.00 30.25	В	C	•
ATOM	7152		AL 174	111. 953	80. 804	25. 125	1.00 30.10	В	0	
ATOM	7153		YS 175	112. 474	79. 990	27. 099	1.00 29.78	В	N	
111 014		., .	110					~	••	

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					(Continued)
				FIG. 4-147	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7154 7155 7156 7157 7158 7159 7160 7161 7162 7163 7164 7165 7166 7167 7177 7172 7173 7174 7175 7176 7177 7178 7177 7178 7179 7180 7181 7182 7183 7184 7185 7186	CA LYS CB LYS CC LYS CC LYS NZ LYS O LYS N ILE CA ILE CB ILE CG ILE CG ILE CG ILE CD ILE CD ILE CD ILE CD ILE CD ILE CD ILE CO ILE CD ILE CD ILE CD ILE CC I	175 175 175 175 175 175 175 176 176 176 176 176 177 177 177 177 177	112. 940 81. 269 27. 608 1. 00 28. 47 B 112. 090 81. 725 28. 794 1. 00 28. 38 B 110. 809 82. 428 28. 413 1. 00 29. 46 B 109. 876 82. 551 29. 611 1. 00 32. 27 B 110. 479 83. 384 30. 725 1. 00 31. 57 B 110. 664 84. 791 30. 307 1. 00 33. 57 B 114. 382 81. 107 28. 064 1. 00 28. 80 B 114. 662 80. 355 28. 999 1. 00 28. 36 B 115. 294 81. 813 27. 401 1. 00 28. 58 B 116. 710 81. 764 27. 749 1. 00 28. 19 B 117. 572 82. 363 26. 624 1. 00 27. 21 B 118. 942 82. 730 27. 146 1. 00 25. 54 B 117. 697 81. 354 25. 483 1. 00 29. 36 B 116. 956 82. 528 29. 044 1. 00 <td>(Continued) C C C C C C C C C C C C C C C C C C</td>	(Continued) C C C C C C C C C C C C C C C C C C
ATOM	7187	CA ASN	179	112.560 88.188 32.021 1.00 37.31 B	C
ATOM	7188	CB ASN	179	113.211 89.329 32.807 1.00 37.54 B	C
ATOM	7189	CG ASN	179	114. 454 89. 860 32. 137 1. 00 37. 86 B	C
ATOM	7190	OD1 ASN	179	115. 419 89. 131 31. 915 1. 00 39. 14 B	O
ATOM	7191	ND2 ASN	179	114. 437 91. 142 31. 806 1. 00 40. 48 B	N
ATOM	7192	C ASN	179	112. 573 88. 540 30. 535 1. 00 36. 88 B	C
ATOM	7193	O ASN	179	112. 205 89. 650 30. 159 1. 00 38. 11 B	O
ATOM	7194	N LEU	180	112. 995 87. 608 29. 689 1. 00 35. 31 B	N
ATOM	7195	CA LEU	180	113.030 87.875 28.260 1.00 34.44 B	C
ATOM	7196	CB LEU	180	114.357 87.417 27.662 1.00 35.92 B	C
ATOM	7197	CG LEU	180	115.621 88.014 28.279 1.00 36.91 B	C
ATOM	7198	CD1 LEU	180	116. 828 87. 572 27. 470 1. 00 37. 09 B	C .
ATOM	7199	CD2 LEU	180	115. 522 89. 536 28. 303 1. 00 37. 24 B	
ATOM	7200	C LEU	180	111. 898 87. 166 27. 547 1. 00 33. 52 B	
ATOM ATOM	7201 7202	O LEU N PRO	180 181	111. 406 86. 149 28. 015 1. 00 32. 50 B 111. 462 87. 704 26. 400 1. 00 34. 20 B	C O N

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					TO I	G = A	_ 1 1 0	1		(Con	tinued)
					ГТ	G. 4	- 148				
ATOM	7203		PRO	181	111.853			1.00 33.21	В	С	
ATOM	7204		PR0	181	110. 373				В	С	
ATOM	7205		PR0	181	110. 337			1.00 33.27	В	С	
ATOM	7206		PRO	181	110.691			1.00 33.21	В	С	
ATOM	7207		PRO	181	110.681	85.608	25.397	1.00 33.03	В	С	
ATOM	7208		PRO	181	111.829	85.180	25.497	1.00 33.18	В	0	
ATOM	7209		SER	182	109.654				В	Ň	
ATOM	7210	CA	SER	182	109.835				B	Č	
ATOM	7211	CB	SER	182	108. 752	82.622			B	Č	
ATOM	7212	0G	SER	182	107. 505			1.00 30.50	B	Ö	
ATOM	7213	С	SER	182	109. 759	83.117	23. 350	1.00 31.89	В	Č	
ATOM	7214	0	SER	182	109.077	83. 812		1.00 33.14	B	Ō	•
ATOM	7215	N	TYR	183	110.463	82.077		1.00 31.53	B	Ň	
ATOM	7216	CA	TYR	183	110. 453	81.677		1.00 30.47	B	C	
ATOM	7217	CB	TYR	183	111.832	81.159		1.00 30.68	B	Č	
ATOM	7218	CG	TYR	183	112.962		21.408	1.00 32.75	B	Č	
ATOM	7219		TYR	183	113.490	82. 235	22.696	1.00 32.39	B	Č	
ATOM	7220		TYR	183	114.517	83.134	22.977	1.00 33.30	B	Č	
ATOM	7221		TYR	183	113. 492	82.926	20.398	1.00 33.06	В	Č	
ATOM	7222		TYR	183	114. 520	83. 832	20.667	1.00 34.20	В	Ċ	
ATOM	7223	CZ	TYR	183	115.028	83. 932	21.959	1.00 34.92	В	Ċ	
ATOM	7224	OH	TYR	183	116.036	84. 832	22. 233	1.00 34.60	В	Ō	
ATOM	7225	C	TYR	183	109. 423	80.568	21.384	1.00 29.28	В	Č	
ATOM	7226	0	TYR	183	109. 387	79.645	22.196	1.00 29.66	В	0	
ATOM	7227	N	ARG	184	108. 579	80.659	20.364	1.00 27.67	В	N	
ATOM	7228	CA	ARG	184	107. 573	79.631	20.148	1.00 26.57	В	C	
ATOM	7229	CB	ARG	184	106.327	80. 217	19.476	1.00 26.06	В	С	
ATOM	7230	CG	ARG	184	105. 215	79. 191	19. 285	1.00 28.64	В	С	
ATOM	7231	CD	ARG	184	103.860	79. 825	19.004	1.00 30.29	В	С	
ATOM	7232	NE	ARG	184	102. 827	78. 805	18.831	1.00 31.47	В	N	
ATOM	7233	CZ	ARG	184	101.526	79.052	18. 706	1.00 29.99	В	C	
ATOM	7234	NH1		184	100.678	78. 048	18. 552	1.00 30.76	В	N	
ATOM	7235	NH2		184	101.068	80. 294	18. 740	1.00 30.05	В	N	
ATOM	7236		ARG	184	108. 185	78. 553	19. 272	1.00 26.51	В	С	
ATOM	7237		ARG	184	108. 375	78. 754	18.072	1.00 28.42	В	0	
ATOM	7238	N	ILE	185	108. 493	77.411	19.876	1.00 24.50	В	N	
ATOM	7239		ILE	185	109.112	76.303	19. 165	1.00 22.88	В	C	
ATOM	7240	CB	ILE	185	109. 773	75.319	20. 159	1.00 23.12	В	С	
ATOM	7241	CG2		185	110.492	74. 216	19.405	1.00 22.56	В	C	
ATOM	7242	CG1		185	110. 753	76.067	21.064	1.00 22.32	В	C	
ATOM	7243	CD1		185	111.869	76.770	20. 324	1.00 21.93	В	C	
ATOM	7244		ILE	185	108. 148	75.516	18. 275	1.00 24.00	В	С	
ATOM	7245		ILE	185	108. 569	74. 930	17. 275	1.00 25.07	В	0	
ATOM	7246		THR	186	106.866	75. 489	18.632	1.00 22.70	В.	N	
ATOM	7247		THR	186	105.886	74. 750		1.00 23.30	В	C	
ATOM	7248		THR	186	105.490	73. 440	18. 541	1.00 22.83	В	С	
ATOM	7249	0G1		186	105.058	73. 727	19.877	1.00 27.42	В	0	
ATOM	7250 7251	CG2 C		186	106.665	72.491		1.00 19.86	В	Č	
ATOM	1441	V	THR	186	104.620	75. 548	17. 537	1.00 23.45	В	C	

					ान	G A	- 1 / 0	\		(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7261 7262 7263 7264	O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 CZ3 CH2	TRP TRP TRP TRP TRP TRP TRP	186 187 187 187 187 187 187 187 187 187 187	104. 266 103. 938 102. 717 103. 007 104. 159 105. 420 103. 041 105. 485 106. 249 105. 723 103. 346 104. 679	75. 179 75. 876 76. 767 76. 767 9 77. 694 8 79. 092 9 79. 548 80. 007 77. 367 78. 474 80. 878 81. 332 81. 751	18. 265 16. 457 16. 049 14. 832 15. 025 15. 321 15. 464 15. 019 15. 298 15. 789 15. 764 15. 922	1. 00 22. 05 1. 00 24. 88 1. 00 25. 32 1. 00 25. 43 1. 00 25. 95 1. 00 26. 07 1. 00 27. 09 1. 00 26. 93 1. 00 26. 08 1. 00 24. 50 1. 00 25. 13	B B B B B B B B B B B B B B B B B B B	O N C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7266 7267 7268 7269 7270 7271 7272 7273 7274 I 7275 7276	O N CA CB OG1 CG2 C O N CA	THR THR THR GLY GLY GLY	187 187 188 188 188 188 188 188 188 189 189	101. 555 100. 481 101. 759 100. 708 101. 304 102. 291 101. 940 99. 817 98. 916 100. 064 99. 278 97. 783	75. 402 73. 636 72. 672	15. 709 15. 339 15. 839 15. 516 14. 895 15. 781 13. 552 16. 687 16. 512 17. 866 19. 045 18. 847	1.00 26.00 1.00 27.74 1.00 26.58 1.00 26.89 1.00 26.63 1.00 27.13 1.00 25.34 1.00 27.17 1.00 26.92 1.00 26.58 1.00 27.32 1.00 28.44	B B B B B B B B	C O N C C O C C O C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7279 (7280 (7281 (7282 (7283 (N I CA I CB I CCB I CCC I CCC I NZ I CCC I NZ I CCC I NCC I	LYS LYS LYS LYS LYS LYS LYS LYS LYS LYS	189 190 190 190 190 190 190 190 191	97. 333 97. 007 95. 554 95. 187 93. 695 93. 498 92. 043 91. 127 94. 815 94. 738 94. 262 93. 516	73. 673 71. 636 71. 686 71. 381 71. 294 71. 031 70. 731 71. 870 70. 731 69. 523 71. 299 70. 558	18. 345 19. 242 19. 085 17. 628 17. 317 15. 821 15. 458 15. 744 20. 028 19. 786 21. 096 22. 110	1.00 30.95 1.00 27.83 1.00 27.15 1.00 29.55 1.00 31.55 1.00 36.65 1.00 39.17 1.00 41.50 1.00 26.61 1.00 25.87 1.00 25.05 1.00 25.10	B B B B B B B	O N C C C C C N C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7289 C 7290 C 7291 C 7292 O 7293 O 7294 C 7295 O 7296 N 7297 C 7298 C 7299 C	CB GCG GCD GCD GCD GCD GCD GCD GCD GCD GCD	LU 1 LU 1 LU 1 LU 1 LU 1 LU 1 LU 1 SP 1 SP 1 SP 1	191 191 191 191 191 191 191 92 92 92	92. 461 91. 821 90. 752 90. 111 90. 551 92. 849 92. 031	71. 475 70. 933 71. 859 71. 522 72. 932 69. 263 69. 280 68. 157 66. 811 66. 733 67. 200 66. 855	22. 728 23. 987 24. 514 25. 536 23. 899 21. 631 20. 713 22. 287 21. 996 22. 149 23. 508	1.00 26.71 1.00 29.36 1.00 34.15 1.00 36.46 1.00 35.96 1.00 23.31 1.00 20.17 1.00 23.70 1.00 24.98 1.00 27.27 1.00 30.85 1.00 32.45	B B B B B B B B	C C C C O O C O N C C C C

					(Continued)
				FIG. 4-150	()
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7301 7302 7303 7304 7305 7306 7307 7308 7309 7310 7311 7312 7313 7314 7315 7316 7317 7318 7319 7320 7321 7322 7323 7324 7325 7326 7327 7328 7329 7330 7331 7332 7331 7332 7333 7334 7335 7336 7337	OD2 ASP C ASP O ASP N ILE CA ILE CB ILE CG1 ILE C ILE C ILE C ILE CA ILE CB ILE CG2 ILE CG1 ILE CG2 ILE CG1 ILE CG2 ILE CG1 IL	192 192 193 193 193 193 193 193 194 194 194 194 195 195 195 195 195 196 196 196 196	## F I G. 4 - 1 5 0 ## 89. 671 67. 908 23. 548 1. 00 32. 44 B 93. 072 66. 329 20. 602 1. 00 25. 95 B 92. 431 65. 426 20. 065 1. 00 27. 81 B 94. 091 66. 926 20. 000 1. 00 25. 46 B 94. 485 66. 512 18. 665 1. 00 25. 50 B 93. 970 67. 502 17. 595 1. 00 26. 97 B 94. 426 67. 057 16. 212 1. 00 26. 11 B 92. 441 67. 552 17. 621 1. 00 27. 90 B 91. 784 66. 246 17. 210 1. 00 29. 23 B 95. 994 66. 390 18. 546 1. 00 25. 04 B 96. 519 65. 297 18. 334 1. 00 26. 34 B 96. 691 67. 510 18. 682 1. 00 22. 43 B 98. 139 67. 505 18. 589 1. 00 21. 47 B 98. 618 68. 429 17. 456 1. 00 21. 58 B 100. 146 68. 414 17. 377 1. 00 18. 60 B 97. 972 68. 001 16. 133 1. 00 19. 45 B 98. 331 66. 613 15. 678 1. 00 15. 81 B 98. 779 67. 968 19. 895 1. 00 21. 61 B 98. 544 69. 095 20. 337 1. 00 22. 13 B 99. 580 67. 095 20. 508 1. 00 19. 09 B 100. 272 67. 429 21. 750 1. 00 18. 17 B 98. 647 65. 941 23. 094 1. 00 21. 37 B 98. 647 65. 941 23. 094 1. 00 21. 37 B 98. 647 65. 941 23. 094 1. 00 20. 38 B 98. 647 65. 942 21. 750 1. 00 18. 17 B 97. 873 65. 269 22. 146 1. 00 20. 38 B 98. 087 66. 187 24. 349 1. 00 20. 45 B 98. 647 65. 968 22. 445 1. 00 20. 38 B 98. 087 66. 187 24. 349 1. 00 21. 55 B 96. 797 65. 768 24. 659 1. 00 20. 48 B 94. 785 64. 650 24. 020 1. 00 19. 77 B 101. 771 67. 579 21. 503 1. 00 18. 27 B 102. 334 68. 710 21. 897 1. 00 17. 52 B 103. 762 68. 941 21. 725 1. 00 17. 52 B 103. 769 69. 311 18. 632 1. 00 17. 04 B 103. 769 69. 311 18. 632 1. 00 17. 01 B	(Continued) O C C C C C C C C C C C C C C C C C C
ATOM ATOM	7338 7339	C ASN O ASN	196 196	104. 380 69. 160 23. 104 1. 00 18. 89 B 103. 976 70. 066 23. 828 1. 00 21. 80 B	C O
ATOM ATOM	7340 7341	N GLY CA GLY	197 197	105. 355 68. 344 23. 479 1. 00 18. 21 B	N
ATOM	7342	C GLY	197	105. 976 68. 533 24. 778 1. 00 18. 42 B 105. 185 67. 948 25. 941 1. 00 18. 43 B	C C
ATOM ATOM	7343 7344	O GLY N ILE	197 198	105. 660 67. 954 27. 088 1. 00 17. 86 B	0
ATOM	7345	CA ILE	198	103. 976 67. 469 25. 654 1. 00 15. 16 B 103. 129 66. 842 26. 667 1. 00 14. 58 B	N C
ATOM ATOM	7346 7347	CB ILE CG2 ILE	198	101.956 67.740 27.160 1.00 12.66 B	C
ATOM	7348	CG2 ILE	198 198	102.477 68.784 28.109 1.00 10.73 B 101.189 68.334 25.970 1.00 14.13 B	C C
ATOM	7349	CD1 ILE	198	99. 936 69. 129 26. 368 1. 00 13. 46 B	C

					(Continued)
				FIG. 4-151	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7350 7351 7352 7353 7354 7355 7356 7357	C ILE O ILE N THR CA THR CB THR OG1 THR CG2 THR C THR	198 198 199 199 199 199 199	102. 523 65. 585 26. 101 1. 00 14. 46 B 102. 354 65. 447 24. 895 1. 00 16. 78 B 102. 182 64. 671 26. 990 1. 00 15. 77 B 101. 600 63. 396 26. 608 1. 00 15. 94 B 101. 982 62. 350 27. 630 1. 00 15. 69 B 101. 683 62. 861 28. 937 1. 00 12. 99 B 103. 473 62. 043 27. 534 1. 00 15. 54 B 100. 085 63. 448 26. 522 1. 00 15. 87 B	0 N C C 0 C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7358 7359 7360 7361 7362 7363 7364	O THR N ASP CA ASP CB ASP CG ASP OD1 ASP OD2 ASP	199 200 200 200 200 200 200 200	99. 452 64. 311 27. 133 1. 00 16. 77 B 99. 510 62. 534 25. 745 1. 00 16. 29 B 98. 058 62. 450 25. 619 1. 00 16. 42 B 97. 654 61. 812 24. 279 1. 00 17. 56 B 97. 960 60. 321 24. 207 1. 00 19. 40 B 98. 894 59. 847 24. 892 1. 00 20. 07 B 97. 267 59. 624 23. 438 1. 00 19. 79 B	N C C
ATOM ATOM ATOM ATOM ATOM ATOM	7365 7366 7367 7368 7369 7370	C ASP O ASP N TRP CA TRP CB TRP CG TRP	200 200 201 201 201 201	97. 657 61. 578 26. 806 1. 00 15. 56 B 98. 502 61. 278 27. 648 1. 00 16. 67 B 96. 404 61. 151 26. 889 1. 00 14. 09 B 96. 003 60. 368 28. 049 1. 00 13. 08 B 94. 503 60. 106 28. 037 1. 00 13. 25 B 94. 023 59. 554 29. 348 1. 00 12. 63 B	C O N C C
ATOM ATOM ATOM ATOM ATOM	7371 7372 7373 7374 7375 7376	CD2 TRP CE2 TRP CE3 TRP CD1 TRP NE1 TRP CZ2 TRP	201 201 201 201 201 201	94. 135 58. 198 29. 801 1. 00 10. 35 B 93. 610 58. 150 31. 110 1. 00 11. 08 B 94. 634 57. 020 29. 228 1. 00 8. 52 B 93. 449 60. 253 30. 370 1. 00 12. 43 B 93. 198 59. 416 31. 434 1. 00 12. 21 B 93. 567 56. 967 31. 858 1. 00 11. 85 B	C C C N C
ATOM ATOM ATOM ATOM ATOM	7377 7378 7379 7380 7381 7382	CZ3 TRP CH2 TRP C TRP O TRP N VAL CA VAL	201 201 201 201 202 202	94. 596 55. 847 29. 968 1. 00 8. 91 B 94. 065 55. 829 31. 271 1. 00 10. 19 B 96. 719 59. 040 28. 264 1. 00 14. 63 B 97. 197 58. 766 29. 366 1. 00 14. 84 B 96. 795 58. 213 27. 224 1. 00 14. 84 B 97. 413 56. 902 27. 369 1. 00 13. 74 B	C C C O N C
ATOM ATOM ATOM ATOM ATOM ATOM	7383 7384 7385 7386 7387 7388	CB VAL CG1 VAL CG2 VAL C VAL O VAL N TYR	202 202 202 202 202 203	97. 028 55. 966 26. 190 1. 00 11. 30 B 97. 960 56. 155 25. 010 1. 00 8. 57 B 97. 028 54. 541 26. 667 1. 00 8. 82 B 98. 929 56. 920 27. 556 1. 00 15. 45 B 99. 471 56. 095 28. 292 1. 00 16. 05 B 99. 616 57. 857 26. 906 1. 00 15. 45 B	C C C C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7389 7390 7391 7392 7393 7394 7395	CA TYR CB TYR CG TYR CD1 TYR CE1 TYR CD2 TYR CE2 TYR	203 203 203 203 203 203 203	101.060 57.941 27.053 1.00 13.39 B 101.656 58.918 26.035 1.00 12.37 B 102.248 58.238 24.823 1.00 8.90 B 101.461 57.938 23.709 1.00 8.82 B 101.989 57.260 22.619 1.00 7.48 B 103.587 57.844 24.812 1.00 5.53 B 104.138 57.167 23.737 1.00 6.51 B	C C C C C
ATOM ATOM ATOM ATOM	7396 7397 7398	CZ TYR OH TYR C TYR	203 203 203 203	104.128 57.167 23.727 1.00 6.51 B 103.325 56.874 22.634 1.00 8.49 B 103.849 56.175 21.572 1.00 8.01 B 101.438 58.371 28.471 1.00 13.68 B	C C O C

					D Î.	· 4 -	1 5 9			(Continued)
					FI(G. 4-	152			
ATOM	7399	0	TYR	203	102. 369	57.832	29.056	1.00 12.65	В	0
ATOM	7400	N	GLU	204	100. 706	59. 335	29.020	1.00 15.26	В	N
ATOM	7401	CA	GLU	204	100.963	59.827	30. 376	1.00 16.69	В	C
ATOM	7402	CB	GLU	204	99. 975	60. 936	30. 743	1.00 16.67	В	C
ATOM	7403	CG	GLU	204	100.174	61.457	32. 161	1.00 17.47	В	.C
ATOM	7404	CD	GLU	204	98. 950	62. 154	32. 731	1.00 17.71	В	C
ATOM	7405	OE1		204	98. 197	62. 785	31.964	1.00 19.00	В	0
ATOM	7406		GLU	204	98. 753	62.085	33. 962	1.00 18.59	В	0
ATOM	7407	C	GLU	204	100. 831 101. 681	58. 740 58. 597	31. 437 32. 305	1.00 17.37 1.00 18.22	B B	C 0
ATOM	7408	0	GLU GLU	204 205	99. 745	57. 980	31.353	1.00 18.22	В	N
ATOM ATOM	7409 7410	N CA	GLU	205	99. 442	56. 932	32. 315	1.00 19.55	В	C
ATOM	7411	CB	GLU	205	97. 925	56.727	32. 344	1.00 20.80	В	č
ATOM	7412	CG	GLU	205	97. 453	55. 436	32. 995	1.00 23.74	В	Č
ATOM	7413	CD	GLU	205	97. 414	55. 494	34. 515	1.00 26.68	В	č
ATOM	7414		GLU	205	97. 038	54. 466	35. 118	1.00 28.71	B	ŏ
ATOM	7415		GLU	205	97. 744	56. 547	35. 106	1.00 26.12	B	Ö
ATOM	7416	C	GLU	205	100. 132	55. 578	32. 131	1.00 19.27	B	Č
ATOM	7417	Ō	GLU	205	100.525	54.957	33.107	1.00 19.31	В	0
ATOM	7418	N	GLU	206	100. 291	55.124	30.893	1.00 18.93	В	N
ATOM	7419	CA	GLU	206	100.876	53.808	30.660	1.00 18.63	В	C
ATOM	7420	CB	GLU	206	99. 989	53.016	29.705	1.00 18.05	В	C
ATOM	7421	CG	GLU	206	98. 535	52.921	30. 139	1.00 20.39	В	C
ATOM	7422	CD	GLU	206	98. 359	52. 143	31.422	1.00 20.74	В	C
ATOM	7423		GLU	206	97. 205	51.905	31.821	1.00 21.45	В	0
ATOM	7424		GLU	206	99. 375	51.768	32.037	1.00 22.90	В	0
ATOM	7425	C	GLU	206	102. 293	53.766	30. 136	1.00 19.32	В	C
ATOM	7426	0	GLU	206	102. 976	52.761	30. 292	1.00 20.01	В	0
ATOM	7427	N	VAL	207	102.744	54. 844	29. 509	1.00 20.90	В	N
ATOM	7428	CA	VAL	207	104.092	54.855	28. 968	1.00 20.95	В	C
ATOM	7429	CB	VAL	207	104. 101	55. 347	27. 509	1.00 21.52	В	C
ATOM	7430		VAL	207	105. 486	55. 151	26. 918	1.00 22.17	В	C
ATOM	7431		VAL	207	103.048	54.592	26. 684 29. 775	1.00 19.10 1.00 21.67	В	C C
MOTA	7432 7433	C 0	VAL VAL	207 207	105. 080 106. 052	55. 691 55. 160	30. 301	1.00 21.07	B B	0
ATOM ATOM	7434	N	PHE	208	100. 032	56. 989	29. 888	1.00 25.52	В	N
ATOM	7435	CA	PHE	208	104. 833	57. 870	30. 611	1.00 21.33	В	C
ATOM	7436	CB	PHE	208	105. 143	59. 201	29. 863	1.00 21.33	В	Č
ATOM	7437	CG	PHE	208	106. 571	59. 083	28. 536	1.00 21.20	В	Č
ATOM	7438		PHE	208	107. 890	58. 649	28. 464	1.00 20.63	В	č
ATOM	7439		PHE	208	105. 893	59. 373	27. 353	1.00 22.58	B	č
ATOM	7440		PHE	208	108. 525	58. 499	27. 230	1.00 22.52	B	č
ATOM	7441		PHE	208	106. 521	59. 225	26. 109	1.00 22.24	B	č
ATOM	7442	CZ	PHE	208	107. 837	58. 787	26. 048	1.00 22.76	B	č
ATOM	7443	Č	PHE	208	105. 444	58. 168	32. 082	1.00 21.89	B	Č
ATOM	7444	Ŏ	PHE	208	106. 298	58. 727	32.768	1.00 23.07	В	0
ATOM	7445	Ň	SER	209	104. 261	57.811	32. 577	1.00 20.48	В	N
ATOM	7446	CA	SER	209	103.922	58.094	33. 976	1.00 19.86	В	С
ATOM	7447	CB	SER	209	104.689	57. 165	34. 905	1.00 18.09	В	C

					(Continued)
				FIG. 4-153	(00
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7448 7449 7450 7451 7452 7453 7454 7455	OG SER C SER O SER N ALA CA ALA CB ALA C ALA O ALA N TYR	209 209 210 210	104. 383 55. 820 34. 601 1. 00 21. 42 B 104. 285 59. 543 34. 286 1. 00 20. 55 B 104. 780 59. 877 35. 367 1. 00 19. 53 B 104. 031 60. 394 33. 302 1. 00 20. 69 B 104. 319 61. 809 33. 393 1. 00 20. 47 B 105. 809 62. 044 33. 228 1. 00 20. 63 B 103. 545 62. 492 32. 275 1. 00 20. 53 B 103. 042 61. 835 31. 367 1. 00 19. 81 B 103. 461 63. 813 32. 354 1. 00 21. 78 B	0 C O N C C C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7457 7458 7459 7460 7461 7462 7463	CA TYR CB TYR CG TYR CD1 TYR CE1 TYR CD2 TYR CE2 TYR	211 211 211 211 211 211 211	102.733 64.634 31.390 1.00 20.95 B 101.944 65.681 32.175 1.00 18.35 B 100.984 66.566 31.411 1.00 15.38 B 100.257 66.086 30.324 1.00 14.13 B 99.310 66.879 29.694 1.00 12.47 B 100.738 67.863 31.846 1.00 11.95 B 99.799 68.657 31.231 1.00 12.21 B	C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7464 7465 7466 7467 7468 7469 7470 7471	CZ TYR OH TYR C TYR O TYR N SER CA SER CB SER OG SER	211 211 211 211 212 212 212 212	99.087 68.165 30.156 1.00 13.68 B 98.158 68.977 29.550 1.00 12.73 B 103.781 65.283 30.508 1.00 22.11 B 103.512 65.742 29.406 1.00 23.55 B 105.000 65.294 31.017 1.00 23.17 B 106.112 65.877 30.310 1.00 22.03 B 107.286 66.055 31.265 1.00 22.38 B 108.441 66.477 30.567 1.00 24.83 B	C O C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7472 7473 7474 7475 7476 7477 7478	C SER O SER N ALA CA ALA CB ALA C ALA O ALA	212 212 213 213 213 213 213 213	106. 547 65. 017 29. 141 1. 00 22. 20 B 106. 651 63. 802 29. 256 1. 00 22. 93 B 106. 791 65. 668 28. 013 1. 00 22. 14 B 107. 267 65. 011 26. 812 1. 00 19. 72 B 106. 157 64. 882 25. 803 1. 00 19. 85 B 108. 360 65. 942 26. 301 1. 00 21. 17 B 108. 443 66. 254 25. 109 1. 00 20. 14 B	C O N C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7479 7480 7481 7482 7483 7484 7485	N LEU CA LEU CB LEU CG LEU CD1 LEU CD2 LEU C LEU	214 214 214 214 214 214 214 214	109. 175 66. 409 27. 243 1. 00 21. 21 B 110. 298 67. 295 26. 961 1. 00 22. 06 B 110. 049 68. 697 27. 534 1. 00 21. 02 B 108. 958 69. 546 26. 878 1. 00 20. 19 B 108. 840 70. 872 27. 603 1. 00 21. 72 B 109. 292 69. 779 25. 426 1. 00 22. 01 B 111. 528 66. 688 27. 615 1. 00 22. 30 B	N C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7486 7487 7488 7489 7490 7491 7492	O LEU N TRP CA TRP CB TRP CG TRP CD2 TRP CE2 TRP	214 215 215 215 215 215 215 215	111. 442 66. 131 28. 703 1. 00 25. 61 B 112. 674 66. 795 26. 957 1. 00 21. 71 B 113. 904 66. 237 27. 497 1. 00 19. 34 B 114. 112 64. 833 26. 942 1. 00 18. 71 B 113. 018 63. 863 27. 294 1. 00 18. 43 B 111. 910 63. 481 26. 468 1. 00 16. 56 B 111. 157 62. 536 27. 194 1. 00 14. 85 B	0 · N C C C C C
ATOM ATOM ATOM ATOM	7493 7494 7495 7496	CE3 TRP CD1 TRP NE1 TRP CZ2 TRP	215 215 215 215 215	111. 482 63. 845 25. 186 1. 00 17. 01 B 112. 890 63. 155 28. 456 1. 00 15. 04 B 111. 781 62. 356 28. 400 1. 00 13. 49 B 109. 996 61. 949 26. 682 1. 00 14. 75 B	C C N C

								(Continued)
			FIG	. 4 -	154			(00000000000000000000000000000000000000
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7500 0 1 7501 N 1 7502 CA 1 7503 CB 1 7504 CG 1 7505 CD2 1 7506 CE2 1 7507 CE3 1 7508 CD1 1 7509 NE1 1 7510 CZ2 1 7511 CZ3 1 7512 CH2 1 7513 C 1	TRP 215 TRP 215 TRP 216	110. 326 109. 599 115. 110 115. 625 115. 566 116. 727 116. 958 116. 020 116. 097 115. 036 116. 959 114. 945 114. 351 114. 815 116. 738 115. 673 117. 982	63. 257 62. 320 67. 096 67. 034 67. 897 68. 743 69. 705 70. 863 72. 099 72. 916 72. 598 70. 974 72. 204 74. 209 73. 887 74. 674 67. 896	24. 675 25. 425 27. 149 26. 028 28. 108 27. 880 29. 048 29. 156 28. 437 28. 896 27. 452 29. 994 29. 844 28. 401 26. 958 27. 435 27. 747	1.00 15.48 1.00 15.57 1.00 20.78 1.00 20.20 1.00 21.49 1.00 22.15 1.00 24.63 1.00 25.56 1.00 25.56 1.00 25.92 1.00 25.92 1.00 24.93 1.00 24.93 1.00 24.95 1.00 23.03	B B B B B B B B B B B B B B B B B B B	C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7515 N S 7516 CA S 7517 CB S 7518 OG S 7519 C S 7520 O S 7521 N P 7522 CD P 7523 CA P 7524 CB P 7524 CB P 7525 CG P	FRP 216 SER 217 SER 217 SER 217 SER 217 SER 217 SER 217 SER 217 SER 218 SER 218	118. 083 118. 941 120. 222 120. 954 121. 212 120. 976 120. 694 121. 942 122. 469 122. 712 123. 961 123. 385 123. 005	66. 816 68. 398 67. 723 68. 223 69. 612 68. 145 69. 198 67. 336 66. 127 67. 646 66. 801 65. 555	28. 334 26. 975 26. 819 25. 575 25. 676 28. 080 28. 656 28. 523 27. 867 29. 727 29. 547 28. 937 30. 010 30. 985	1. 00 21. 32 1. 00 25. 91 1. 00 26. 96 1. 00 28. 77 1. 00 31. 27 1. 00 27. 00 1. 00 26. 90 1. 00 26. 67 1. 00 26. 69 1. 00 27. 32 1. 00 26. 93 1. 00 27. 70 1. 00 30. 37	B B B B B B B B B B B B B B B B B B B	O N C C O C O N C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7528 N A 7529 CA A 7530 CB A 7531 CG A 7532 OD1 A 7533 ND2 A 7534 C A 7535 O A 7536 N G 7537 CA G 7538 C G 7539 O G 7540 N T 7541 CA T 7542 CB T 7542 CB T 7543 OG1 T 7544 CG2 T	SN 219 SN 219 SN 219 SN 219 SN 219 SN 219 SN 219 SN 219 LY 220 LY 220 LY 220 LY 220 HR 221 HR 221 HR 221	123. 818 124. 129 125. 485 125. 447 124. 376 126. 626 123. 029 123. 212 121. 888 120. 765 120. 823 120. 097 121. 669 121. 775 123. 052 124. 213 123. 068 7	69. 770 71. 176 71. 562 71. 562 71. 640 71. 725 71. 632 72. 133 73. 351 71. 575 72. 391 73. 030 73. 986 72. 512 73. 073 72. 584 73. 084	29. 184 29. 435 28. 816 27. 308 26. 706 26. 690 28. 958 28. 943 28. 565 28. 137 26. 765 26. 500 25. 884 24. 547 23. 808 24. 481 22. 367	1.00 27.72 1.00 26.82 1.00 26.61 1.00 27.23 1.00 25.21 1.00 30.87 1.00 27.38 1.00 26.98 1.00 26.98 1.00 26.91 1.00 27.55 1.00 27.00 1.00 26.99 1.00 27.74 1.00 29.49 1.00 26.25 1.00 26.42	B B B B B B B B B B B B B B B B B B B	N C C C O N C C O C C C C C C C C C C C

				FIG. 4	- 155			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7558 7559 7560 7561 7562 7563 7564 7565 7566 7567 7568 7569 7571 7572 7573 7574 7575 7576 7577 7578 7577 7578 7579 7580 7581 7582 7583 7584 7585	O THR PHE CA PHE CB PHE CCD PHE CCD PHE CCD PHE CCD PHE CCD PHE CCD LEU CCD TYR CCA TYR CCB TYR CCB TYR CCB TYR CCD TY	221 222 222 222 222 222 222 222 222 223 223 223 223 223 223 223 223 224 224	119. 862 73. 551 120. 305 71. 386 119. 158 70. 923 119. 480 69. 644 120. 722 69. 723 121. 955 69. 384 120. 661 70. 113 123. 115 69. 428 121. 815 70. 158 123. 046 69. 814 117. 949 70. 618 118. 066 70. 282 116. 780 70. 746 115. 540 70. 442 114. 618 71. 667 113. 248 71. 340 113. 469 70. 684 112. 389 72. 587 114. 885 69. 380 114. 462 69. 650 114. 834 68. 162 114. 935 65. 776 112. 761 66. 968 114. 935 65. 776 112. 761 66. 968 114. 935 66. 755 110. 423 66. 635 110. 423 66. 635 110. 680 69. 443 110. 680 69. 443 110. 607 70. 017 108. 543 68. 399 108. 466 68. 970 109. 502 69. 777	23. 201 23. 619 22. 850 22. 069 21. 246 21. 797 19. 912 21. 031 19. 132 19. 693 23. 723 24. 901 23. 789 23. 878 24. 503 25. 860 24. 644 22. 934 21. 808 23. 248 24. 444 22. 328 23. 248 24. 444 22. 328 23. 248 24. 444 22. 328 23. 248 24. 328 24. 444 22. 328 23. 248 24. 328 24. 328 25. 703 26. 607 27. 701 21. 332 20. 849 19. 589 19. 589 19. 244 18. 796 17. 553 21. 737 20. 607 22. 195 21. 381 22. 173	1. 00 28. 29 1. 00 25. 34 1. 00 25. 65 1. 00 26. 36 1. 00 26. 35 1. 00 26. 12 1. 00 28. 19 1. 00 28. 19 1. 00 24. 55 1. 00 24. 55 1. 00 24. 55 1. 00 21. 81 1. 00 22. 85 1. 00 21. 10 1. 00 21. 10 1. 00 23. 23 1. 00 23. 23 1. 00 23. 23 1. 00 23. 37 1. 00 23. 38 1. 00 24. 27 1. 00 23. 38 1. 00 23. 37 1. 00 23. 38 1. 00 24. 27 1. 00 23. 38 1. 00 24. 27 1. 00 23. 38 1. 00 24. 27 1. 00 23. 38 1. 00 24. 27 1. 00 18. 49 1. 00 18. 49 1. 00 21. 31 1. 00 18. 23 1. 00 22. 86 1. 00 14. 89 1. 00 14. 89 1. 00 14. 89 1. 00 19. 66 1. 00 19. 66 1. 00 19. 19 1. 00 19. 73	B B B B B B B B B B B B B B B B B B B	(Continued) O N C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM	7587 7588 7589 7590	O ALA N GLN CA GLN CB GLN CG GLN	226 227 227 227 227 227	106. 107 65. 908 105. 912 64. 410 104. 659 64. 968 104. 823 65. 709 103. 512 66. 300	21.576 1 19.909 1 19.457 1 18.139 1	1. 00 21. 22 1. 00 16. 70 1. 00 17. 01 1. 00 17. 47 1. 00 18. 65	B B B B	O N C C
ATOM ATOM ATOM	7592 7593	CD GLN OE1 GLN NE2 GLN	227 227 227 227	103. 554 66. 788 103. 724 66. 007 103. 394 68. 090	16. 249 1 15. 320 1	1.00 18.45 1.00 18.91 1.00 19.57	B B B	C O N

ATOM

7643

CG1 VAL

233

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(Continued) FIG. 4-156 19.274 GLN 227 103.651 63.841 1.00 17.21 ATOM 7595 C 0 103.931 62.850 18.594 1.00 17.76 В 7596 0 GLN 227 ATOM 1.00 16.03 63.990 19.888 В N N PHE 228 102.483 ATOM 7597 1.00 17.64 C В PHE 228 101.447 62.980 19.768 ATOM 7598 CA C 228 100.985 62.524 21.158 1.00 14.78 В 7599 PHE CB**ATOM** PHE 228 102.111 62.105 22.065 1.00 13.03 В C CG ATOM 7600 1.00 12.33 PHE 228 102.659 63.003 22.982 В C ATOM CD1 7601 102.653 21.978 C 60.826 1.00 12.01 В CD2 PHE 228 ATOM 7602 C 228 103.732 62.636 23.796 1.00 9.77 В CE1 PHE 7603 **ATOM** C CE2 PHE 103.725 60.450 22.786 1.00 11.27 В 228 7604 ATOM 23.698 9.50 C 104.267 61.360 В PHE 228 1.00 **ATOM** 7605 CZĊ 63.523 18.955 1.00 18.96 В PHE 228 100.263 **ATOM** 7606 C 99.894 64.697 19.064 1.00 19.98 В 0 7607 0 PHE 228 **ATOM** 229 99.685 62.657 18.133 1.00 20.11 В N ASN 7608 N ATOM 98.548 63.002 17.285 1.00 20.74 C В 229 **ATOM** 7609 CA ASN 98.965 62.867 15.819 1.00 22.98 B C ASN 229 7610 CB **ATOM** 97.980 14.867 1.00 27.56 В C ASN 229 63.488 7611 CG ATOM 96.795 63.610 15.174 1.00 31.63 В 0 229 7612 OD1 ASN ATOM 98.467 63.871 13.692 1.00 30.76 В N ATOM 7613 ND2 ASN 229 229 97.435 61.995 17.609 1.00 21.10 В C ATOM 7614 ASN C 17.283 ATOM ASN 229 97.550 60.816 1.00 20.02 В 0 7615 0 96. 369 95. 277 18.260 1.00 22.16 ASP 230 62.444 ATOM 7616 N В N 18.608 61.534 1.00 24.31 В C ATOM 7617 CA **ASP** 230 7618 CB **ASP** 230 94.877 61.683 20.079 1.00 23.86 В C ATOM 7619 CG **ASP** 230 95.999 61.332 21.027 1.00 25.25 В C **ATOM** 22.159 OD1 ASP 60.914 ATOM 7620 230 95.701 1.00 27.89 В 0 20.656 **ATOM** 7621 OD2 ASP 230 97.180 61.485 1.00 27.78 В 0 7622 61.776 17.740 **ATOM** C ASP 230 94.0561.00 24.83 В C 92. 927 94. 297 7623 ASP 61.496 18.148 1.00 24.00 230 В ATOM 0 0 62.284 1.00 25.37 7624 THR 231 16.536 **ATOM** N В N 93.229 7625 62.582 15.593 1.00 26.24 **ATOM** CA THR 231 B C 93.802 231 62.868 14.193 1.00 25.71 C 7626 THR В ATOM CB 94. 439 14.194 1.00 26.78 0 ATOM 7627 0G1 THR 231 64.151 В Ċ 92.702 ATOM 7628 CG2 THR 231 62.851 13.150 1.00 23.72 В 92.148 61.510 15.467 **ATOM** 7629 C THR 231 1.00 27.04 В C 90.964 61.815 15.604 1.00 29.05 ATOM 7630 0 THR 231 В 0 60. 265 15.211 1.00 27.00 7631 232 92.545 ATOM N **GLU** В N 7632 CA 91.574 59.183 15.038 1.00 26.30 ATOM GLU 232 В C CB 92.017 58.286 13.877 1.00 29.71 В C ATOM 7633 GLU 232 7634 CG 59.036 12.563 ATOM GLU 232 92.177 1.00 36.71 В ATOM 58.253 7635 CD GLU 232 92.971 11.519 1.00 39.94 B C 7636 92.434 57.273 10.943 **ATOM** OE1 GLU 232 1.00 41.61 B 0 OE2 GLU 7637 232 94.142 58.623 11.286 1.00 39.28 В ATOM 0 58. 328 7638 91.32016.282 1.00 23.78 В C **ATOM** C **GLU** 232 7639 90.683 57.280 16.208 1.00 23.18 **ATOM** 0 GLU 232 В 0 7640 91.823 1.00 21.91 ATOM N VAL 233 58.763 17.427 В N C ATOM 7641 CA VAL 233 91.608 58.010 18.652 1.00 20.18 B ATOM 7642 CB VAL 233 92.651 58.375 19.727 1.00 20.26 В C

57.627 SUBSTITUTE SHEET (RULE 26)

21.016

1.00 18.23

B

92.352

				FIG. 4-157	(Continued)
ATOM	7644		233	94. 050 58. 032 19. 223 1. 00 18. 80 B	С
ATOM	7645		233	90. 218 58. 339 19. 175 1. 00 18. 04 B	С
ATOM	7646		233	89. 886 59. 507 19. 378 1. 00 19. 49 B	0
ATOM	7647		234	89. 383 57. 315 19. 394 1. 00 16. 04 B	N
ATOM ATOM	7648		234	89. 633 55. 876 19. 231 1. 00 14. 37 B	C
ATOM	7649 7650		234	88. 025 57. 544 19. 896 1. 00 15. 33 B	C
ATOM	7651	CG PRO	$\begin{array}{c} 234 \\ 234 \end{array}$	87. 461 56. 133 20. 030 1. 00 13. 91 B	C
ATOM	7652		234	88. 247 55. 363 19. 013 1. 00 12. 89 B 88. 048 58. 275 21. 227 1. 00 14. 45 B	C
ATOM	7653		234	88. 048 58. 275 21. 227 1. 00 14. 45 B 89. 043 58. 242 21. 950 1. 00 13. 13 B	C 0
ATOM	7654		235	86. 941 58. 927 21. 547 1. 00 14. 92 B	N N
ATOM	7655	CA LEU	235	86. 831 59. 676 22. 791 1. 00 13. 91 B	Č
ATOM	7656	CB LEU	235	86. 131 61. 005 22. 536 1. 00 14. 93 B	č
ATOM	7657	CG LEU	235	86. 627 61. 937 21. 434 1. 00 16. 83 B	č
ATOM	7658	CD1 LEU	235	85. 581 63. 030 21. 198 1. 00 17. 90 B	č
ATOM	7659	CD2 LEU	235	87. 963 62. 534 21. 833 1. 00 14. 85 B	č
ATOM	7660	C LEU	235	85. 998 58. 911 23. 803 1. 00 12. 70 B	Č
ATOM	7661	O LEU	235	84. 941 58. 385 23. 456 1. 00 13. 27 B	0
ATOM	7662	N ILE	236	86. 468 58. 801 25. 039 1. 00 10. 71 B	N
ATOM	7663	CA ILE	236	85. 618 58. 165 26. 037 1. 00 10. 96 B	C C
ATOM	7664	CB ILE	236	86. 385 57. 630 27. 283 1. 00 9. 70 B	С
ATOM ATOM	7665 7666	CG2 ILE	236	87. 316 58. 692 27. 859 1. 00 10. 05 B	C
ATOM	7667	CG1 ILE CDI ILE	$\begin{array}{c} 236 \\ 236 \end{array}$	85. 386 57. 246 28. 371 1. 00 7. 51 B	C
ATOM	7668	CDI ILE	236	84. 465 56. 100 28. 002 1. 00 9. 77 B 84. 774 59. 369 26. 456 1. 00 12. 91 B	C
ATOM	7669	0 ILE	236	A = A = A = A = A = A = A = A = A = A =	C
ATOM	7670	N GLU	237	85. 277 60. 500 26. 486 1. 00 13. 64 B 83. 497 59. 156 26. 741 1. 00 13. 69 B	0 N
ATOM	7671	CA GLU	237	82. 651 60. 267 27. 150 1. 00 14. 30 B	N C
ATOM	7672	CB GLU	237	81. 657 60. 643 26. 041 1. 00 15. 93 B	Č .
ATOM	7673	CG GLU	237	82. 307 60. 993 24. 708 1. 00 20. 06 B	Č
ATOM	7674	CD GLU	237	81. 311 61. 541 23. 682 1. 00 24. 67 B	č
ATOM	7675	OE1 GLU	237	80. 133 61. 125 23. 713 1. 00 27. 11 B	Ŏ
ATOM	7676	OE2 GLU	237	81. 706 62. 377 22. 832 1. 00 25. 71 B	0
ATOM	7677	C GLU	237	81. 902 59. 898 28. 407 1. 00 12. 26 B	C
ATOM	7678	O GLU	237	81. 473 58. 759 28. 569 1. 00 12. 02 B	0
ATOM ATOM	7679 7680	N TYR	238	81. 768 60. 860 29. 310 1. 00 12. 67 B	N
ATOM	7681	CA TYR CB TYR	238	81. 044 60. 630 30. 550 1. 00 13. 08 B	C
ATOM	7682	CG TYR	238 238	81. 903 59. 816 31. 534 1. 00 11. 88 B	C
ATOM	7683	CD1 TYR	238	83. 201 60. 458 31. 954 1. 00 15. 20 B 83. 250 61. 347 33. 026 1. 00 15. 46 B	C
ATOM	7684	CE1 TYR	238	04 450 04 000	C
ATOM	7685	CD2 TYR	238	04 000 00 100	C
ATOM	7686	CE2 TYR	238	84. 390 60. 160 31. 291 1. 00 14. 07 B 85. 592 60. 727 31. 683 1. 00 14. 24 B	C
ATOM	7687	CZ TYR	238	85. 623 61. 606 32. 751 1. 00 13. 94 B	C C
ATOM	7688	OH TYR	238	86. 818 62. 173 33. 129 1. 00 12. 45 B	Ö
ATOM	7689	C TYR	238	80. 583 61. 944 31. 163 1. 00 13. 53 B	Č
ATOM	7690	O TYR	238	81. 095 63. 008 30. 832 1. 00 14. 88 B	Ŏ
ATOM	7691	N SER	239	79. 592 61. 865 32. 042 1. 00 14. 64 B	Ň
ATOM	7692	CA SER	239	79.040 63.047 32.684 1.00 13.89 B	C
				01 ID 07 IT IT 01 ID 01	

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					17	· T C	· 1		1 5 0				(Continued)	
					r	1 (у. 4	-	158						
ATOM	7693	CB	SER	239		. 597	62. 78		33. 085		13. 29	В		C	
ATOM	7694	0G	SER	239		. 800	62. 49		31.961		19.37	В		0	
ATOM	7695	C	SER	239		. 775	63. 54		33. 915		14.65	В		C	
ATOM	7696	0	SER	239		. 361	62. 77		34. 673		15.52	В		0	
ATOM	7697	N	PHE	240		. 737	64. 86		34. 100		14.89	В		N	
ATOM	7698	CA	PHE	240		. 313	65. 49		35. 276		15.60	В		C	
ATOM	7699	CB	PHE	240		. 543	66. 32		34. 932		17.00	В		C	
ATOM	7700	CC	PHE	240		. 422 . 325	66. 59 65. 62		36. 112 36. 547		14.96	B B		C C	
ATOM ATOM	7701 7702		PHE PHE	240 240		. 312	67. 78		36. 822		15.66	В		C	
ATOM	7703		PHE	240		. 108	65. 84		37. 675		13.32	В		Č	
ATOM	7704		PHE	240		. 087	68.00		37. 950		12.45	В		Č	
ATOM	7705	CZ	PHE	240		. 988	67. 03		38. 379		11.23	В		Č	
ATOM	7706	C	PHE	240		. 184	66. 40		35. 758		15.75	В		Č	
ATOM	7707	ŏ	PHE	240		. 671	67. 23		34. 995		14.05	В		ŏ	
ATOM	7708	Ň	TYR	241		. 785	66. 23		37. 013		15.13	$\tilde{\mathtt{B}}$		N	
ATOM	7709	CA	TYR	241		683	67.00		37. 567		14. 92	B		Ċ	
ATOM	7710	CB	TYR	241		912	66.12		38. 545		13. 15	B		Č	
ATOM	7711	CG	TYR	241		480	64.84		37.880		12.77	В		Ċ	
ATOM	7712	CD1	TYR	241		. 393	64.83		37.007	1.00	11.36	В		C	
ATOM	7713	CE1	TYR	241	75.	. 051	63.67		36. 304		12.47	В		C	
ATOM	7714		TYR	241		. 215	63.67		38.041	1.00	12.85	В		C	
ATOM	7715		TYR	241		. 883	62.51		37. 342		12.55	В		C	
ATOM	7716	CZ	TYR	241		801	62.52		36. 472		12.41	В		C	
ATOM	7717	OH	TYR	241		489	61.39		35. 748		12.90	В		0	
ATOM	7718	C	TYR	241		. 100	68. 29		38. 208		15. 24	В		C	
ATOM	7719	0	TYR	241		311	69. 23		38. 263		17.04	В		0	
ATOM	7720	N	SER	242		. 337	68. 35		38. 694		16.92	В		N	
ATOM	7721	CA	SER	242		864	69.57		39. 305		16.89	В		C	
ATOM	7722	CB	SER	242		816	70.70		38. 280		15.48	В		C	
ATOM	7723 7724	OG C	SER	242		439	71.87		38. 782		18. 12	В		0	
ATOM ATOM	7725	0	SER SER	242 242		078	69.96		40.548		16.70	В		C	
ATOM	7726	N	ASP	242	70	. 438 . 136	69.12 71.24	1 '	41. 171 40. 912		18. 07 17. 57	B B		O N	
ATOM	7727	CA	ASP	243 243		405	71.72		42. 075		19. 72	. В		C	
ATOM		CB	ASP	243		846			42. 442			В		C	
ATOM	7729	CG	ASP	243		275	73. 18		42. 950		28. 70	В		C	
ATOM	7730	0D1		243		646	72.30		43. 765		29.62	В		0	
ATOM	7731	OD2		243		021	74.10		42. 542		29.69	В		0	
ATOM	7732	C	ASP	243		917	71.70		41.772		20. 24	В		Č	
ATOM	7733	Ŏ	ASP	243		508	71.77		10.609		20. 38	В		Ŏ	
ATOM	7734	N	GLU	244		104	71.62		12.818		19. 25	B		N	
ATOM	7735	CA	GLU	244		668	71.54		12.630		19. 29	B		Ċ	
ATOM	7736	CB	GLU	244		966	71.37		13.988		19.46	B		Č	
ATOM	7737	CG	GLU	244		283	72.60		14. 533		23.65	B		č	
ATOM	7738	CD	GLU	244		567	72. 33		15.847		26.30	В		Č	
ATOM	7739	0E1	GLU	244		225	71.85		16.797	1.00	28.64	В		Ō	
ATOM	7740	0E2.		244		349	72. 59	5 4	15. 934		27.72	В		0	
ATOM	7741	C	GLU	244	74.	086	72.72		11.850	1.00	18.30	В		С	

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					TO 1 C	1 -	160			(Continued)
					FIG	. 4 -				
ATOM	7791		YS ·	250	84. 262	70.465	31.442	1.00 26.19	В	N .
ATOM	7792		YS	250	79. 215	67. 313	31.040	1.00 17.64	В	C 0
ATOM	7793		YS	250	79.348	66. 409	31.867 29.750	1.00 20.20 1.00 15.06	B B	N N
ATOM	7794		THR	251	79. 478 79. 978	67. 160 65. 905	29. 234	1.00 13.00	В	Č
ATOM	7795		THR THR	251 251	79. 317	65. 537	27. 896	1.00 13.86	В	č
ATOM ATOM	7796 7797		THR	251	77. 965	65. 144	28. 128	1.00 14.97	B	Ö
ATOM	7798		THR	251	80. 058	64. 389	27. 227	1.00 13.23	В	C
ATOM	7799		THR	251	81.473	66.016	29.015	1.00 15.66	В	C
ATOM	7800		THR	251	81.934	66.831	28. 227	1.00 18.88	В	0
ATOM	7801		/AL	252	82. 231	65. 194	29. 720	1.00 15.28	В	N
ATOM	7802		/AL	252	83.675	65. 195	29. 578	1.00 15.13	В	C
ATOM	7803		VAL	252	84. 335	64. 717	30. 882	1.00 13.64	В	C
ATOM	7804	CG1 V		252	85. 827	64. 580	30. 706	1.00 10.22	B B	C C
ATOM	7805	CG2 V		252	84.012	65. 701 64. 264	31. 991 28. 422	1.00 11.83 1.00 17.21	В	Č
ATOM	7806		VAL	$\begin{array}{c} 252 \\ 252 \end{array}$	84. 027 83. 472	63. 173	28. 304	1.00 17.21	В	ő
ATOM ATOM	7807 7808		VAL ARG	252 253	84. 929	64. 710	27. 557	1.00 18.91	B	Ň
ATOM	7809		ARG	253	85. 349	63. 922	26. 403	1.00 20.46	B	Ċ
ATOM	7810		ARG	253	84. 822	64. 560	25. 113	1.00 22.21	В	С
ATOM	7811		ARG	253	83. 399	64. 137	24.755	1.00 26.72	В	C
ATOM	7812		ARG	253	82.847	64.920	23. 578	1.00 28.87	В	С
ATOM	7813		ARG	253	82. 176	66. 132	24.033	1.00 36.20	В	N
ATOM	7814		ARG	253	80. 870	66. 221	24. 278	1.00 38.47	В	C
ATOM	7815	NH1 A		253	80. 084	65. 164	24. 099	1.00 39.84	В	N N
ATOM	7816	NH2		253	80. 352	67. 360	24. 727 26. 389	1.00 37.97 1.00 19.71	B B	C
ATOM	7817		ARG	253 253	86. 863 87. 520	63. 863 64. 886	26. 246	1.00 13.11	В	Ö
ATOM	7818 7819		ARG VAL	253 254	87. 404	62.656	26. 538	1.00 18.34	В	Ň
ATOM ATOM	7820		VAL	254	88. 847	62. 434	26. 594	1.00 15.15	B	Ċ
ATOM	7821		VAL	254	89. 257	61.924	27. 994	1.00 16.16	В	Č
ATOM	7822	CG1		254	90. 771	61.759	28.081	1.00 15.18	В	C
ATOM	7823	CG2		254	88. 736	62.868	29.065	1.00 16.46	В	C
ATOM	7824		VAL	254	89. 313	61.397	25. 585	1.00 14.67	В	C
ATOM	7825		VAL	254	88. 806	60. 272	25. 566	1.00 14.87	В	0
ATOM	7826		PRO	255	90. 281	61.757	24. 726	1.00 13.62	В	N
ATOM	7827		PRO	255	90. 872	63.081	24. 472	1.00 12.90	B B	C .
ATOM	7828		PRO	255	90. 760	60.777	23. 746 22. 933	1.00 12.62 1.00 11.40	В	C
ATOM	7829		PRO PRO	255 255	91.786 91.263	61.566 62.969	23. 013	1.00 11.40	В	Č
ATOM ATOM	7830 7831		PRO	255 255	91. 203	59.645	24. 553	1.00 12.46	B	č
ATOM	7832		PRO	255	92. 355	59. 831	25. 282	1.00 13.25	B	Ŏ
ATOM	7833		TYR	256	90. 796	58. 469	24. 414	1.00 12.53	B	N
ATOM	7834		TYR	256	91. 217	57. 306	25. 161	1.00 12.05	В	С
ATOM	7835		TYR	256	90. 319	57. 205	26. 398	1.00 12.42	В	C C
ATOM	7836		TYR	256	90. 608	56.082	27. 360	1.00 14.53	В	Ç
ATOM	7837		TYR	256	91.021	56. 355	28.662	1.00 16.44	В	C
ATOM	7838			256	91. 192	55. 337	29. 596	1.00 17.38	В	C
ATOM	7839	CD2	TYR	256	90. 382	54. 752	27. 010	1.00 15.31	В	C

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						(Continued)
					FIG. 4-161	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7840 7841 7842 7843 7844 7845 7846 7847 7850 7851 7852 7853 7856 7857 7858 7859 7860 7861 7862 7863 7864 7865 7866 7867 7868 7869 7870 7871 7872 7873 7874 7875 7876 7877 7878 7879 7879	CZ OH C O N CDA CC C O N CC C C O N CC C C C	VAL	256 256 256 256 257 257 257 257 257 257 257 258 258 258 258 258 259 260 260 261 261 262 262 262 262 262 262 262 262	90. 548 53. 724 27. 941 1. 00 16. 91 B 90. 949 54. 030 29. 232 1. 00 16. 54 B 91. 068 53. 042 30. 176 1. 00 17. 03 B 91. 040 56. 094 24. 263 1. 00 11. 63 B 89. 923 55. 765 23. 870 1. 00 13. 76 B 92. 141 55. 415 23. 924 1. 00 10. 78 B 93. 535 55. 786 24. 231 1. 00 9. 21 B 92. 098 54. 229 23. 068 1. 00 9. 97 B 93. 473 54. 233 22. 438 1. 00 8. 95 B 94. 326 54. 657 23. 606 1. 00 8. 91 B 91. 859 52. 949 23. 869 1. 00 11. 12 B 92. 694 52. 556 24. 681 1. 00 9. 90 B 90. 723 52. 300 23. 648 1. 00 11. 97 B 90. 444 51. 057 24. 353 1. 00 13. 52 B 88. 930 50. 855 24. 492 1. 00 15. 66 B 88. 305 51. 808 25. 522 1. 00 14. 41 B 86. 801 51. 730 25. 552 1. 00 18. 08 B 86. 204 52. 655 26. 627 1. 00 19. 12 B 86. 355 52. 156 28. 030 1. 00 14. 62 B 91. 101 49. 934 23. 571 1. 00 14. 62 B 91. 101 49. 934 23. 571 1. 00 14. 64 B 91. 227 48. 760 24. 178 1. 00 16. 07 B 91. 227 48. 760 24. 178 1. 00 16. 07 B 91. 247 47. 627 23. 515 1. 00 14. 32 B 91. 476 47. 476 22. 045 1. 00 16. 09 B 90. 293 47. 415 21. 710 1. 00 15. 64 B 92. 477 47. 428 21. 172 1. 00 15. 95 B 91. 841 48. 523 18. 982 1. 00 17. 08 B 91. 781 48. 488 17. 752 1. 00 18. 87 B 91. 198 50. 851 18. 983 1. 00 14. 62 B 91. 198 50. 851 18. 983 1. 00 17. 08 B 92. 221 47. 269 19. 673 1. 00 14. 62 B 91. 198 50. 851 18. 983 1. 00 17. 08 B 92. 379 51. 509 18. 292 1. 00 17. 12 B 93. 489 50. 986 18. 292 1. 00 17. 12 B 93. 489 50. 986 18. 292 1. 00 17. 12 B 93. 489 50. 986 18. 292 1. 00 17. 12 B 93. 489 50. 986 18. 292 1. 00 17. 12 B 93. 489 50. 986 18. 292 1. 00 17. 12 B 93. 489 50. 986 18. 292 1. 00 17. 12 B 93. 489 50. 986 18. 292 1. 00 17. 12 B 93. 489 50. 986 18. 292 1. 00 17. 12 B 93. 489 50. 986 18. 292 1. 00 17. 12 B 93. 489 50. 986 18. 292 1. 00 17. 12 B 93. 489 50. 986 18. 292 1. 00 17. 12 B 93. 489 50. 986 18. 292 1. 00 17. 12 B 93. 192 53. 384 17. 004 1. 00 16. 00 B 92. 614 54. 371 15. 947 1. 00 14. 51 B 93. 717 55. 252 15. 383 1. 00 13. 59 B 91. 970 53. 596 14. 820 1. 00 10. 82	(Continued) C C C C C C C C C C C C C C C C C C
ATOM	7878	CG1	VAL	262	93. 717 55. 252 15. 383 1. 00 13. 59 B	C
ATOM ATOM	7880 7881	C	VAL VAL	262 262	93. 984 54. 150 18. 055 1. 00 17. 31 B	С
ATOM ATOM	7882 7883	N	ASN ASN	263 263	95. 275 53. 856 18. 128 1. 00 16. 87 B	0 N
ATOM ATOM	7884 7885	CB	ASN ASN	263 263	97. 406 53. 595 19. 292 1. 00 17. 58 B	C C
ATOM ATOM	7886 7887	OD1 ND2	ASN	263 263	97. 230 52. 629 20. 437 1. 00 20. 08 B 97. 919 51. 606 20. 500 1. 00 19. 88 B 96. 329 52. 950 21. 365 1. 00 18. 44 B	C 0
ATOM	7888		ASN	263	96. 329 52. 950 21. 365 1. 00 18. 44 B 96. 706 55. 827 18. 533 1. 00 18. 01 B	N C

					(Continued)
				FIG. 4-162	Conninuou
ATOM ATOM ATOM	7889 7890 7891	O ASN N PRO CD PRO	263 264 264	97. 288 56. 646 19. 413 1. 00 17. 06 I 97. 357 56. 546 20. 883 1. 00 15. 68 I	B O B N B C
ATOM ATOM	7892 7893	CA PRO	264 264		ВС
ATOM	7894	CG PRO	264	98. 411 57. 569 21. 214 1. 00 14. 78	B C B C
ATOM	7895	C PRO	264		ВС
ATOM ATOM	7896 7897	O PRO N THR	264 265	99. 669 56. 527 18. 369 1. 00 15. 27 99. 560 58. 521 17. 354 1. 00 16. 21	
ATOM	7898	CA THR	265	100. 796 58. 305 16. 617 1. 00 15. 30 F	
ATOM	7899	CB THR	265	100. 647 58. 677 15. 132 1. 00 15. 20 H	
ATOM ATOM	7900 7901	OG1 THR CG2 THR	265 265	100.081 59.983 15.029 1.00 17.05 E 99.747 57.687 14.415 1.00 10.60 E	
ATOM	7902	C THR	265	101. 818 59. 211 17. 279 1. 00 16. 13	
ATOM	7903	0 THR	265	101. 454 60. 126 18. 007 1. 00 16. 83	3 0
ATOM ATOM	7904 7905	N VAL CA VAL	266 266	103.095 58.971 17.030 1.00 17.64 E 104.118 59.781 17.667 1.00 17.49	
ATOM	7906	CB VAL	266	104.116 35.181 17.007 1.00 17.49 1	
ATOM	7907	CG1 VAL	266	105. 224 57. 714 18. 538 1. 00 12. 10 E	3 C
ATOM	7908	CG2 VAL	266	105.642 59.921 19.666 1.00 12.62 E	
ATOM ATOM	7909 7910	C VAL 0 VAL	266 266	105. 312 60. 112 16. 769 1. 00 19. 23 E 105. 693 59. 331 15. 893 1. 00 18. 24 E	
ATOM	7911	N LYS	267	105. 889 61. 287 17. 003 1. 00 20. 19	
ATOM	7912	CA LYS	267	107. 058 61. 756 16. 272 1. 00 19. 42 B	3 C
ATOM ATOM	7913 7914	CB LYS	$\frac{267}{267}$	106. 678 62. 855 15. 291 1. 00 19. 76 E 105. 786 62. 413 14. 168 1. 00 21. 59 E	
ATOM	7915	CD LYS	267	105. 452 63. 605 13. 291 1.00 23. 15	
ATOM	7916	CE LYS	267	104. 593 63. 205 12. 119 1. 00 23. 47 B	3 C
ATOM	7917	NZ LYS	267	104. 225 64. 402 11. 334 1. 00 27. 20 B	
ATOM ATOM	7918 7919	C LYS O LYS	267 267	108. 032 62. 334 17. 288 1. 00 19. 59 B 107. 618 62. 826 18. 336 1. 00 20. 86 B	
ATOM	7920	N PHE	268	109. 322 62. 275 16. 984 1. 00 19. 32 B	
ATOM	7921	CA PHE	268	110.325 62.818 17.882 1.00 18.94 B	B C
ATOM ATOM	7922 7923	CB PHE	268 268	111. 350 61. 757 18. 259 1. 00 17. 47 B 112. 186 62. 131 19. 444 1. 00 16. 21 B	
ATOM	7924	CD1 PHE	268	112. 186 62. 131 19. 444 1. 00 16. 21 B 111. 601 62. 290 20. 692 1. 00 16. 98 B	
ATOM	7925	CD2 PHE	268	113. 555 62. 327 19. 313 1. 00 16. 35 B	-
ATOM	7926	CE1 PHE	268	112. 368 62. 639 21. 797 1. 00 18. 80 B	
ATOM ATOM	7927 7928	CE2 PHE CZ PHE	268 268	114. 332 62. 674 20. 405 1. 00 17. 68 B 113. 737 62. 832 21. 655 1. 00 18. 66 B	
ATOM	7929	C PHE	268	111.016 63.979 17.192 1.00 20.34 B	
ATOM	7930	0 PHE	268	111.114 64.016 15.968 1.00 21.73 B	0
ATOM	7931 7932	N PHE CA PHE	269 269	111. 491 64. 931 17. 981 1. 00 20. 76 B	
ATOM ATOM	7933	CB PHE	269 269	112. 152 66. 105 17. 435 1. 00 20. 74 B 111. 141 67. 239 17. 222 1. 00 19. 80 B	
ATOM	7934	CG PHE	269	110.070 66.937 16.216 1.00 21.88 B	C
ATOM	7935	CD1 PHE	269	110. 332 67. 019 14. 853 1. 00 22. 75 B	C
ATOM ATOM	7936 7937	CD2 PHE CE1 PHE	269 269	108. 785 66. 605 16. 631 1. 00 23. 20 B 109. 326 66. 781 13. 912 1. 00 21. 98 B	
711 Om	1001	ODI III	200	100.020 UU. (OI 10.312 1.UU 21.30 D	U

		ī	rig. 4	-163			(Continued)
ATOM 793 ATOM 794 ATOM 795 ATOM 796 ATOM 7970 ATOM 7970 ATOM 7971 ATOM 7972 ATOM 7973 ATOM 7974 ATOM 7974 ATOM 7978 ATOM 7980 ATOM 7981 ATOM 7984 ATOM 7984 ATOM 7984 ATOM 7984	9 CZ PHE 1 O PHE 2 N VAL 3 CA VAL 4 CB VAL 5 CG1 VAL 6 CG2 VAL 7 C VAL 8 O VAL 9 N VAL 9 N VAL 9 CA VAL 1 CB VAL 2 CG1 VAL 1 CB VAL 2 CG1 VAL 3 CG2 VAL 4 C VAL 6 N ASN 7 CA ASN 8 CG ASN 8 CG ASN 9 OD1 ASN 9 ND2 ASN 9 ND3 THR 9 CA THR 9 CG1 THR 9 CG2 THR	269 107 269 108 269 113 269 113 270 114 270 115 270 116 270 115 271 115 271 114 271 114 271 114 271 114 271 117 272 118 272 121 272 121 272 121 272 121 272 121 272 121 272 121 272 121 272 121 273 118 273 118 273 118 273 118 274 121 274 121 274 121 274 121 275 120 275 120 275 120 275 1	951 74.056 179 74.672 094 75.706 330 74.036 347 75.104 943 76.012 397 75.208 938 76.411 509 76.100 653 75.727 510 74.960 988 77.516 78.139 671 77.446 019 77.049 047 76.363 267 77.430 277 78.996 389 80.058 78.542 176 79.279 186 79.279 187 79.652 180 79.355	4 15. 700 1. 4 14. 337 1. 5 18. 402 1. 6 19. 613 1. 7 18. 58 1. 1 18. 667 1. 1 18. 635 1. 1 19. 630 1. 1 18. 985 1. 1 18. 985 1. 1 18. 973 1. 1 18. 714 1. 20. 177 1. 18. 186 1. 19. 363 1. 20. 536 1. 19. 363 1. 20. 536 1. 19. 383 1. 20. 536 1. 19. 383 1. 21. 292 1. 21. 292 1. 21. 292 1. 21. 292 1. 21. 292 1. 21. 292 1. 21. 292 1. 21. 292 1. 21. 292 1. 21. 292 1. 21. 292 1. 21. 292 1. 21. 292 1. 21. 292 1. 21. 292 1. 21. 292 1. 21. 292 1. 21. 293 1. 22. 208 1. 21. 696 1. 21. 775 1. 22. 208 1. 23. 403 1. 24. 181 1. 23. 403 1. 21. 676 1. 21. 775 1. 20. 419 1. 20. 366 1. 21. 775 1. 20. 366 1. 21. 775 1. 20. 366 1. 21. 775 1. 21. 698 1. 22. 208 1. 23. 193 1. 24. 117 1. 20. 419 1. 20. 366 1. 21. 775 1. 21. 698 1. 22. 208 1. 23. 193 1. 24. 117 1. 25. 419 1. 26. 419 1. 27. 751 1. 28. 166 1. 29. 17. 751 1. 29. 17. 751 1. 20. 366 1. 20	00 23. 06 00 22. 44 00 21. 66 00 21. 27 00 23. 26 00 23. 10 00 23. 57 00 23. 02 00 25. 32 00 26. 96 00 27. 45 00 27. 39 00 27. 39 00 27. 39 00 27. 43 00 27. 43 00 27. 43 00 27. 43 00 27. 45 00 27. 46 00 31. 23 00 32. 45 00 32. 45 00 33. 79 00 34. 53 00 35. 53 00 37. 39 00 34. 53 00 37. 39 00 34. 53 00 37. 39 00 38. 58 00 39. 58 00 40. 66	888888888888888888888888888888888888888	(Continued) C C C C C C C C C C C C C C C C C C
ATOM 7986	CA LEU	276 116.		18. 443 1. 00	0 40.56 0 40.53	B B	N C

					FIG	S. 4-	164			(Continued)
ATOM ATOM	7987 7988	CG 1	LEU 2	76 76	116. 076 116. 002	80. 425 78. 958	19.664 20.097	1.00 38. 1.00 36.	34 B	С
ATOM ATOM ATOM	7989 7990 7991	CD1 I CD2 I C	LEU 2	76 76 76	115. 319 115. 261 116. 914	78. 876 78. 134 82. 229	21. 445 19. 057 18. 140	1. 00 35. 1. 00 32. 1. 00 41.	57 B	C
ATOM ATOM ATOM	7992 7993 7994	N :	SER 2	76 77 77	117. 675 116. 029 115. 916	83. 002 82. 634 84. 044	18. 721 17. 233 16. 863	1.00 41. 1.00 44. 1.00 46.	02 B	N
ATOM ATOM	7995 7996	CB S	SER 2 SER 2	77 77	116. 489 116. 268	84. 277 85. 618	15. 462 15. 044	1.00 48. 1.00 50.	49 B 90 B	C 0
ATOM ATOM ATOM	7997 7998 7999	0	SER 2	77 77 78	114. 494 113. 529 114. 378	84. 586 83. 856 85. 884	16. 902 16. 701 17. 148	1.00 46. 1.00 46. 1.00 46.	82 B	0
ATOM ATOM ATOM	8000 8001 8002	CB	SER 2	78 78 78	113. 081 113. 204 113. 617	86. 535 87. 899 87. 759	17. 202 17. 884 19. 234	1.00 47. 1.00 48. 1.00 49.	09 B	C C 0 ·
ATOM ATOM	8003 8004	C :	SER 2 SER 2	78 78 79	112. 531 111. 325	86. 710 86. 829 86. 723	15. 794 15. 600 14. 808	1.00 48. 1.00 48. 1.00 48.	26 B 73 B	C 0
ATOM ATOM ATOM	8005 8006 8007	CA 'CB	VAL 2 VAL 2	79. 79	113. 419 112. 995 114. 189	86. 889 87. 229	13. 428 12. 514	1.00 48. 1.00 49.	89 B 95 B	N C C
ATOM ATOM ATOM	8008 8009 8010	CG1 V CG2 V	VAL 2	79 79 79	113. 709 114. 902 112. 340	87. 454 88. 464 85. 606	11.089 13.037 12.941	1. 00 50. 1. 00 50. 1. 00 48.	28 B	C C C
ATOM ATOM ATOM	8011 8012 8013	N	THR 2	79 80 80	111. 130 113. 145 112. 651	85. 433 84. 708 83. 432	13. 082 12. 380 11. 872	1. 00 49. 1. 00 47. 1. 00 46.	70 B	O N C
ATOM ATOM	8014 8015	CB COG1	THR 2 THR 2	80 80	113. 719 113. 179	82. 709 81. 479	11. 032 10. 531	1.00 47. 1.00 48.	86 B 07 B	C 0
ATOM ATOM ATOM	8018	0 1	THR 2 THR 2	80 80 80	114. 946 112. 238 112. 586	82. 399 82. 484 82. 677	11. 883 12. 992 14. 155	1. 00 47. 1. 00 45. 1. 00 44.	40 B 24 B	C C O
ATOM ATOM ATOM	8019 8020 8021	CA I	ASN 2	81 81 81	111. 499 111. 040 109. 744	81. 447 80. 454 79. 815	12. 622 13. 581 13. 089	1.00 45. 1.00 44. 1.00 46.	81 B	N C C
ATOM ATOM ATOM	8022 8023 8024	CG A OD1 A ND2 A	ASN 2	81 81 81	108. 592 108. 351 107. 873		13. 096 14. 101 11. 984	1. 00 48. 1. 00 49. 1. 00 52.	62 B	C O N
ATOM ATOM	8025 8026	C 1	ASN 2 ASN 2	81 81	112. 088 112. 874	79. 379 79. 065	13. 812 12. 919	1. 00 43. 1. 00 44.	47 B 44 B	C 0
ATOM ATOM ATOM	8027 8028 8029	CA A	ALA 2 ALA 2	82 82 82	112. 100 113. 045 112. 795	77. 773 77. 301	15. 019 15. 371 16. 792	1. 00 41. 1. 00 38. 1. 00 37.	62 B 75 B	N C C
ATOM ATOM ATOM	8030 8031 8032	0 /	ALA ·2 THR 2	82 82 83	112. 863 111. 797 113. 905		14. 403 13. 815 14. 231	1. 00 37. 1. 00 36. 1. 00 36.	86 B	C O N
ATOM ATOM ATOM	8033 8034 8035		THR 2	83 83 83	113. 828 114. 867 114. 665	74. 672 74. 772 75. 994	13. 335 12. 218 11. 495	1. 00 35. 1. 00 37. 1. 00 41.	70 B	C C O

					FI	G. 4	-165	.		(Continued)
ATOM	8036	CG2	THR	283					Th.	C
ATOM	8037	C	THR	283	114.736				В	C
ATOM		Õ	THR	283 283	114.074				В	C
ATOM	8039	N	SER	284	115.098				В	0
ATOM	8040	CA	SER	284 284	113. 123				В	N
ATOM	8040	CB	SER	284	113. 250				В	C
ATOM		OG	SER	284 284	111.935 111.722				В	C
ATOM		C	SER	284	111. 722				В	0
ATOM		Ö	SER	284 284	113.003				В	C .
ATOM		N	ILE	285	114. 684				В	0 N
ATOM		CA	ILE	285 285	115. 130				В	N C
ATOM		CB	ILE	285	116. 660				В	C
ATOM			ILE	285	117. 103				. B	C
ATOM			ILE	285	117. 383	69. 350				C
ATOM			ILE	285 285	117. 303	70. 303			В	C
ATOM		C	ILE	285	114. 429	66. 996	14. 428 13. 976	1.00 34.47 1.00 28.14	В	C
ATOM		Õ	ILE	285	114. 472	66.694	15. 168	1.00 28.14	В	C
ATOM		N	GLN	286	113. 775	66. 278	13. 108	1.00 30.23	В В	0 N
ATOM		CA	GLN	286	113.067	65. 076		1.00 23.84	В	N
ATOM		CB	GLN	286	111.852	64. 886		1.00 24.81	В	C
ATOM		CG	GLN	286	111.169	63. 547		1.00 23.81		C
ATOM			GLN	286	109. 928	63. 417	11.868	1.00 23.29	B B	C
ATOM		0E1		286	109. 253	62. 388	11.894	1.00 25.36	В	C
ATOM		NE2		286	109. 614	64. 461	11.110	1.00 23.22	В	0 N
ATOM			GLN	286	113. 955	63. 838	13. 386	1.00 25.74	В	C
ATOM			GLN	286	114. 832	63. 732	12. 526	1.00 26.39	В	0
ATOM			ILE	287	113. 723	62. 908	14. 307	1.00 24.54	В	N
ATOM			ILE	287	114. 458	61.655	14. 346	1.00 23.40	В	C
ATOM		CB	ILE	287	115. 193	61. 481	15. 694	1.00 21.87	В	C
ATOM		CG2		287	115. 925	60. 143	15. 728	1.00 20.61	В	C
ATOM		CG1		287	116. 180	62. 632	15. 887	1.00 19.27	В	C
MOTA		CD1	ILE	287	117.054	62.506	17. 113	1.00 20.58	В	C
ATOM			ILE	287	113. 394	60. 578	14. 186	1.00 24.59	В	Č
ATOM			ILE	287	112. 729	60. 204	15. 142	1.00 27.03	В	0
ATOM			THR	288	113. 219	60. 093	12.966	1.00 25.43	В	N
ATOM	8071		THR	288	112. 205	59. 088	12. 708	1.00 26.10	В	Č
ATOM	8072		THR	288	111.964			1.00 26.69	B	č
ATOM	8073 (0G1	THR	288	113. 172	58. 516	10. 539	1.00 26.37	В	0
ATOM		CG2		288	111.510	60. 255	10. 593	1.00 25.25	B	Č
ATOM			THR	288	112. 529	57. 741	13. 335	1.00 26.85	В	Č
ATOM	8076 (THR	288	113.687	57.379	13. 503	1.00 27.04	B	Ö
ATOM	8077 N		ALA	289	111.484	57.011	13. 702	1.00 28.37	B	N
ATOM	8078 (ALA	289	111.638	55.705	14. 325	1.00 27.90	B	Č
ATOM			ALA	289	110.271	55.151	14.710	1.00 26.91	B	C C
ATOM			ALA	289	112. 348	54.740	13.380	1.00 27.44	B	č
ATOM	8081 () /	ALA	289	112.550	55.038	12. 205	1.00 28.30	B	ŏ
ATOM	8082 N		PRO	290	112.758	53.577	13.895	1.00 26.01	B	Ň
ATOM			PRO	290	112.903	53. 280	15. 328	1.00 24.74	B	Ċ
ATOM	8084 (CA I	PRO	290	113. 445	52.569		1.00 25.29	B	č
				e.	IDSTITUTE			•	_	-

						(Continued)
					FIG. 4-166	(Convinued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8085 8086 8087 8088 8089 8090 8091 8092 8093 8094 8095 8096	CB CG C O N CA CB C O N CA	PRO PRO PRO ALA ALA ALA ALA SER SER SER	290 290 290 290 291 291 291 291 291 292 292	113. 949 51. 587 14. 138 1. 00 25. 76 B 114. 151 52. 467 15. 342 1. 00 25. 10 B 112. 465 51. 931 12. 110 1. 00 25. 85 B 111. 255 51. 961 12. 330 1. 00 25. 95 B 112. 988 51. 345 11. 038 1. 00 25. 39 B 112. 143 50. 730 10. 024 1. 00 26. 17 B 112. 987 50. 271 8. 846 1. 00 26. 28 B 111. 337 49. 568 10. 573 1. 00 27. 18 B 110. 203 49. 331 10. 145 1. 00 27. 46 B 111. 916 48. 843 11. 521 1. 00 27. 54 B 111. 220 47. 704 12. 103 1. 00 28. 19 B 112. 161 46. 892 12. 993 1. 00 28. 00 B	C C C O N C C C O N C
ATOM ATOM ATOM	8097 8098 8099	0G C 0	SER SER SER	292 292 292	112.525 47.626 14.145 1.00 32.22 B 110.027 48.182 12.922 1.00 28.13 B 109.176 47.376 13.307 1.00 29.52 B	0 C 0
ATOM ATOM ATOM	8100 8101 8102	N CA CB	MET MET MET	293 293 293	109. 976 49. 487 13. 190 1. 00 25. 00 B 108. 881 50. 072 13. 955 1. 00 24. 80 B 109. 387 51. 173 14. 892 1. 00 24. 61 B	N C C C
ATOM ATOM ATOM ATOM	8103 8104 8105 8106	CG SD CE C	MET MET MET MET	293 293 293 293	110. 231 50. 703 16. 060 1. 00 26. 88 B 109. 323 49. 647 17. 189 1. 00 27. 80 B 110. 457 48. 319 17. 438 1. 00 25. 74 B 107. 836 50. 677 13. 027 1. 00 24. 57 B	S C C
ATOM ATOM ATOM	8107 8108 8109	O N CA	MET LEU LEU	293 294 294	106. 641 50. 528 13. 252 1. 00 25. 32 B 108. 292 51. 360 11. 983 1. 00 24. 37 B 107. 393 52. 008 11. 041 1. 00 23. 80 B	O N C
ATOM ATOM ATOM	8110 8111 8112	CB CG	LEU LEU LEU	294 294 294 294	108. 183 52. 930 10. 114 1. 00 23. 40 B 108. 945 54. 072 10. 786 1. 00 24. 87 B 109. 806 54. 787 9. 758 1. 00 22. 08 B	C C C
ATOM ATOM ATOM	8113 8114 8115		LEU LEU LEU	294 294 294 294	107. 958 55. 037 11. 440 1. 00 23. 08 B 106. 540 51. 059 10. 204 1. 00 23. 95 B 105. 714 51. 510 9. 422 1. 00 25. 36 B	C C 0
ATOM ATOM ATOM	8116 8117 8118	N CA CB	ILE ILE ILE	295 295 295 295	106. 724 49. 754 10. 357 1. 00 23. 92 B 105. 923 48. 812 9. 580 1. 00 25. 26 B 106. 601 47. 444 9. 453 1. 00 26. 06 B	N C C
ATOM ATOM ATOM	8119 8120 8121	CG2 CG1 CD1	ILE ILE ILE	295 295 295	107. 972 47. 595 8. 812 1. 00 26. 54 B 106. 698 46. 796 10. 831 1. 00 24. 44 B 107. 211 45. 388 10. 789 1. 00 28. 37 B	C C C
ATOM ATOM ATOM ATOM	8122 8123 8124 8125	C O N CA	ILE ILE GLY GLY	295 295 296 296	104. 564 48. 575 10. 221 1. 00 26. 01 B 103. 805 47. 712 9. 775 1. 00 28. 75 B 104. 263 49. 328 11. 273 1. 00 24. 77 B 102. 992 49. 167 11. 951 1. 00 22. 28 B	C O N C
ATOM ATOM ATOM	8126 8127 8128	C O N	GLY GLY ASP ASP	296 296 297	102. 908 50. 040 13. 182 1. 00 21. 29 B 103. 820 50. 818 13. 447 1. 00 20. 80 B 101. 818 49. 920 13. 935 1. 00 20. 38 B 101. 654 50. 718 15. 141 1. 00 20. 14 B	C O N C
ATOM ATOM ATOM ATOM ATOM	8129 8130 8131 8132 8133		ASP ASP ASP ASP	297 297 297 297 297	101. 034 50. 718 13. 141 1. 00 20. 14 B 100. 366 50. 339 15. 874 1. 00 21. 58 B 99. 109 50. 665 15. 078 1. 00 22. 60 B 98. 016 50. 234 15. 502 1. 00 25. 00 B 99. 200 51. 350 14. 041 1. 00 22. 18 B	C C O O

				FIG. 4-167	(Continued)
ATOM	8134	C ASP	297	102.845 50.481 16.065 1.00 20.31 B	С
ATOM	8135	0 ASP	297	103.419 49.390 16.096 1.00 20.82 B	0
ATOM	8136	N HIS	298	103. 220 51. 508 16. 814 1. 00 16. 87 B	N
ATOM	8137	CA HIS	298	104. 335 51. 384 17. 734 1. 00 16. 48 B	C
ATOM	8138	CB HIS	298	105.669 51.399 16.968 1.00 14.91 B	C
ATOM	8139	CG HIS	298	105.868 52.628 16.137 1.00 12.24 B	C
ATOM	8140	CD2 HIS	298	106. 539 53. 775 16. 391 1. 00 10. 39 B	C
ATOM	8141	ND1 HIS	298	105. 264 52. 802 14. 909 1. 00 11. 35 B	N
ATOM	8142	CE1 HIS	298	105.551 54.005 14.445 1.00 11.25 B	С
ATOM	8143	NE2 HIS	298	106. 323 54. 616 15. 326 1. 00 11. 96 B	N
ATOM	8144	C HIS	298	104. 274 52. 560 18. 693 1. 00 15. 84 B	C
ATOM	8145	0 HIS	298	103. 484 53. 476 18. 505 1. 00 17. 04 B	0
ATOM	8146	N TYR	299	105. 127 52. 539 19. 706 1. 00 15. 50 B	N
ATOM	8147	CA TYR	299	105.163 53.599 20.698 1.00 15.35 B	C
ATOM	8148	CB TYR	299	104. 640 53. 095 22. 047 1. 00 14. 51 B	С
ATOM	8149	CG TYR	299	103. 343 52. 320 22. 037 1. 00 14. 30 B	C C C
ATOM	8150	CD1 TYR	299	102. 120 52. 973 21. 942 1. 00 13. 49 B	C
ATOM	8151	CE1 TYR	299	100. 924 52. 269 22. 019 1. 00 15. 63 B	С
ATOM	8152	CD2 TYR	299	103. 341 50. 933 22. 198 1. 00 14. 56 B	C
ATOM	8153	CE2 TYR	299	102.150 50.216 22.273 1.00 15.40 B	С
ATOM	8154	CZ TYR	299	100. 943 50. 891 22. 186 1. 00 15. 73 B	C
ATOM	8155	OH TYR	299	99. 756 50. 197 22. 286 1. 00 15. 37 B	0
ATOM	8156	C TYR	299	106. 583 54. 084 20. 952 1. 00 16. 54 B	C
ATOM	8157	O TYR	299	107. 559 53. 364 20. 732 1. 00 15. 53 B	0
ATOM	8158	N LEU	300	106. 688 55. 316 21. 428 1. 00 16. 67 B	N
ATOM	8159	CA LEU	300	107. 975 55. 853 21. 818 1. 00 17. 75 B	C
ATOM	8160	CB LEU	300	107. 986 57. 367 21. 654 1. 00 18. 54 B	C
ATOM	8161	CG LEU	300	109. 238 58. 059 22. 183 1. 00 20. 06 B	C
ATOM ATOM	8162 8163	CD1 LEU CD2 LEU	300	110.449 57.535 21.429 1.00 20.50 B	C
ATOM	8164	CDZ LEU	300	109.107 59.567 22.024 1.00 20.10 B	C
ATOM	8165	0 LEU	300 300	107. 897 55. 477 23. 294 1. 00 18. 55 B 106. 894 55. 783 23. 935 1. 00 20. 71 B	C
ATOM	8166	N CYS	301		0
ATOM	8167	CA CYS	301		N
ATOM	8168	CB CYS	301	108. 788 54. 418 25. 252 1. 00 20. 22 B 108. 582 52. 907 25. 375 1. 00 20. 55 B	C
ATOM	8169	SG CYS	301	100.002 52.507 23.575 1.00 20.55 B	C S
ATOM	8170		301	109. 895 54. 842 26. 194 1. 00 20. 82 B	S C
ATOM	8171	0 CYS	301	109.816 54.579 27.395 1.00 21.62 B	0
ATOM	8172	N ASP	302	110.922 55.496 25.662 1.00 22.13 B	N
ATOM	8173	CA ASP	302	112.035 55.968 26.481 1.00 20.03 B	C
ATOM	8174	CB ASP	302	112.875 54.810 27.014 1.00 20.49 B	č
ATOM	8175	CG ASP	302	114. 035 55. 296 27. 868 1. 00 25. 77 B	č
ATOM	8176	OD1 ASP	302	113.880 55.344 29.109 1.00 26.02 B	Ö
ATOM	8177	OD2 ASP	302	115.097 55.664 27.297 1.00 27.73 B	ŏ
ATOM	8178	C ASP	302	112.959 56.894 25.711 1.00 20.08 B	č
ATOM	8179	0 ASP	302	113. 367 56. 596 24. 586 1. 00 19. 30 B	Ŏ
ATOM	8180	N VAL	303	113. 302 58. 010 26. 343 1. 00 20. 41 B	N
ATOM	8181	CA VAL	303	114.188 59.000 25.756 1.00 20.36 B	Ċ
ATOM	8182	CB VAL	303	113. 435 60. 316 25. 470 1. 00 19. 97 B	č
					-

				FIG. 4-168	((Continued)
4 500 1	0100	001 VAI	000		В	С
ATOM	8183	CG1 VAL	303	114.387 61.347 24.857 1.00 20.23 112.260 60.043 24.540 1.00 17.52	В	č
ATOM	8184	CG2 VAL	303 303	115. 267 59. 251 26. 788 1. 00 21. 02	В	č
ATOM	8185 8186	C VAL O VAL	303	114. 950 59. 568 27. 939 1. 00 19. 39	B	ŏ
ATOM ATOM	8187	N THR	304	116.536 59.112 26.389 1.00 21.38	B	N
ATOM	8188	CA THR	304	117.639 59.313 27.332 1.00 21.48	В	C
ATOM	8189	CB THR	304	118.008 58.002 28.046 1.00 19.77	В	С
ATOM	8190	OG1 THR	304	116. 869 57. 496 28. 751 1. 00 19. 55	В	0
ATOM	8191	CG2 THR	304	119.136 58.242 29.026 1.00 20.57	В	C
ATOM	8192	C THR	304	118. 925 59. 851 26. 729 1. 00 22. 96	В	C
ATOM	8193	0 THR	304	119.579 59.159 25.952 1.00 25.30	В	0
ATOM	8194	N TRP	305	119.307 61.069 27.102 1.00 22.41	В	N
ATOM	8195	CA TRP	305	120. 545 61. 643 26. 583 1. 00 21. 86	В	C
ATOM	8196	CB TRP	305	120. 696 63. 114 26. 975 1. 00 20. 21	В	C
ATOM	8197	CG TRP	305	119. 682 64. 002 26. 354 1. 00 18. 90	В	C
ATOM	8198	CD2 TRP	305	119. 834 64. 751 25. 150 1. 00 18. 79	В	C
ATOM	8199	CE2 TRP	305	118.614 65.413 24.917 1.00 20.14	В	C C
ATOM	8200	CE3 TRP	305	120. 885 64. 928 24. 243 1. 00 18. 65 118. 414 64. 232 26. 794 1. 00 17. 49	B B	C
ATOM	8201	CD1 TRP	305	• • • • • • • • • • • • • • • • • • • •	В	N
ATOM	8202	NE1 TRP	305	117. 764 65. 077 25. 938 1. 00 18. 37 118. 413 66. 242 23. 812 1. 00 19. 16	В	Č
ATOM	8203	CZ2 TRP	305 305	120. 689 65. 746 23. 152 1. 00 19. 59	В	Č
ATOM	8204	CZ3 TRP CH2 TRP	305	119. 459 66. 395 22. 943 1. 00 21. 43	В	č
ATOM ATOM	8205 8206	CHZ TRP	305	121.722 60.875 27.148 1.00 22.21	B	č
ATOM	8207	0 TRP	305	121.743 60.552 28.338 1.00 21.63	B	Ŏ
ATOM	8208	N ALA	306	122.697 60.591 26.285 1.00 22.53	В	N
ATOM	8209	CA ALA	306	123.899 59.864 26.673 1.00 21.31	В	C
ATOM	8210	CB ALA	306	124.350 58.969 25.533 1.00 20.65	В	С
ATOM	8211	C ALA	306	124.975 60.882 27.000 1.00 21.97	В	С
ATOM	8212	0 ALA	306	125.675 60.767 28.007 1.00 20.32	В	0
ATOM	8213	N THR	307	125.086 61.885 26.133 1.00 23.85	В	N
ATOM	8214	CA THR	307	126.057 62.964 26.284 1.00 24.42	В	C
ATOM	8215	CB THR	307	127. 285 62. 744 25. 411 1. 00 22. 67	В	C
ATOM	8216	OG1 THR	307	126. 894 62. 855 24. 040 1. 00 25. 33	В	0
ATOM	8217	CG2 THR	307	127. 892 61. 374 25. 659 1. 00 19. 34	В	C
ATOM	8218	C THR	307	125. 397 64. 250 25. 812 1. 00 25. 73	В	C
ATOM	8219	0 THR	307	124. 177 64. 326 25. 731 1. 00 28. 17	В	0 N
ATOM	8220	N GLN	308	126. 210 65. 249 25. 479 1. 00 26. 09	В	N C
ATOM	8221	CA GLN	308	125.699 66.540 25.022 1.00 24.49 126.762 67.634 25.175 1.00 22.95	B B	C
ATOM	8222	CB GLN	308		В	Č
ATOM	8223	CG GLN	308 308	127. 301 67. 811 26. 574 1. 00 21. 20 . 126. 256 68. 296 27. 548 1. 00 20. 30	В	Č
ATOM	8224 8225	CD GLN OE1 GLN	308	126. 477 68. 290 28. 754 1. 00 23. 08	B	ŏ
ATOM ATOM	8226	NE2 GLN	308	125. 116 68. 727 27. 032 1. 00 21. 02	В	Ň
ATOM	8227	C GLN	308	125. 284 66. 501 23. 569 1. 00 25. 09	B	Ċ
ATOM	8228	O GLN	308	124.612 67.411 23.095 1.00 26.23	B	Ö
ATOM	8229	N GLU	309	125. 687 65. 459 22. 855 1. 00 25. 59	B	Ñ
ATOM	8230	CA GLU	309	125.370 65.374 21.440 1.00 26.16	В	С
ATOM	8231	CB GLU	309	126.581 65.807 20.627 1.00 25.99	В	С
0	-201	420				

ATOM 8232 CG GLU 309 126.925 67.280 20.774 1.00 29.27 B C ATOM 8233 CD GLU 309 128.243 67.637 20.109 1.00 31.48 B C ATOM 8234 OEI GLU 309 128.8614 66.968 19.115 1.00 33.35 B O ATOM 8235 OE2 GLU 309 128.909 68.593 20.572 1.00 32.54 B O ATOM 8236 C GLU 309 124.939 63.991 21.004 1.00 26.83 B C ATOM 8237 O GLU 309 124.850 63.712 19.806 1.00 28.64 B O ATOM 8238 N ARG 310 124.674 63.131 21.982 1.00 25.93 B N ATOM 8239 CA ARG 310 124.674 63.131 21.982 1.00 24.07 B C ATOM 8240 CB ARG 310 125.357 60.790 22.121 1.00 24.28 B C ATOM 8241 CG ARG 310 125.5012 59.317 21.952 1.00 24.00 B C ATOM 8242 CD ARG 310 125.525 58.469 22.132 1.00 24.02 B C ATOM 8243 NE ARG 310 127.225 58.790 21.097 1.00 25.36 B N ATOM 8244 CZ ARG 310 127.225 58.790 21.097 1.00 25.36 B N ATOM 8244 CZ ARG 310 129.956 58.063 22.298 1.00 26.17 B N ATOM 8245 NHI ARG 310 129.956 58.063 22.382 1.00 26.60 B N ATOM 8248 NHZ ARG 310 129.956 68.663 61.607 23.757 1.00 26.60 B N ATOM 8249 N ILE 311 120.663 60.843 22.491 1.00 20.40 B C ATOM 8249 N ILE 311 120.663 60.843 22.491 1.00 20.40 B C ATOM 8249 N ILE 311 120.922 61.124 21.829 1.00 23.55 B C ATOM 8249 N ILE 311 119.586 61.607 23.757 1.00 23.67 B N ATOM 8250 CA ILE 311 119.5663 60.843 22.491 1.00 20.40 B C ATOM 8251 CB ILE 311 119.586 61.866 22.879 1.00 18.56 B C ATOM 8252 CC2 ILE 311 119.586 61.866 22.879 1.00 18.52 B C ATOM 8253 CG1 ILE 311 119.586 61.866 22.879 1.00 18.52 B C ATOM 8256 C ILE 311 120.663 60.843 22.491 1.00 20.40 B C ATOM 8257 N SER 312 119.889 56.355 23.837 1.00 21.75 B N ATOM 8258 CA SER 312 119.889 56.355 23.837 1.00 21.75 B N ATOM 8256 C ILE 311 120.663 60.843 22.491 1.00 20.40 B C ATOM 8256 C ILE 311 17.758 56.575 25.132 1.00 21.54 B N ATOM 8257 N SER 312 119.889 56.355 23.837 1.00 21.75 B N ATOM 8258 CA SER 312 119.889 56.355 23.837 1.00 21.75 B N ATOM 8256 C ILE 311 118.305 61.666 22.879 1.00 21.54 B N ATOM 8257 N SER 312 119.588 56.542 22.882 1.00 23.75 B C ATOM 8268 CD SER 312 119.588 56.540 20.754 1.00 21.93 B N ATOM 8269 C B SER 312 119.588 56.866 20.754 1.00 21.93 B N ATOM 8269 C LE
ATOM 8270 O LEU 313 115.868 54.209 21.293 1.00 22.55 B O ATOM 8271 N GLN 314 114.167 54.579 22.722 1.00 22.54 B N ATOM 8272 CA GLN 314 113.666 53.216 22.639 1.00 23.08 B C ATOM 8273 CB GLN 314 113.682 52.549 24.012 1.00 22.45 B C ATOM 8274 CG GLN 314 115.065 52.459 24.626 1.00 25.62 B C ATOM 8275 CD GLN 314 115.092 51.630 25.898 1.00 26.36 B C ATOM 8276 0E1 GLN 314 114.835 50.428 25.870 1.00 27.68 B O ATOM 8277 NE2 GLN 314 115.403 52.273 27.023 1.00 25.65 B N ATOM 8278 C GLN 314 112.242 53.240 22.083 1.00 23.35 B C ATOM 8279 O GLN 314 111.412 54.045 22.513 1.00 22.96 B O ATOM 8280 N TRP 315 111.984 52.372 21.108 1.00 22.35 B N

				F	ΙG	. 4 -	170	•			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8281 8282 8283 8284 8285 8286 8287 8290 8291 8292 8293 8294 8295 8296 8297 8298 8300 8301 8302 8303 8304 8305 8306 8307 8308 8310 8311 8312 8313 8314 8315 8316 8317 8318 8319 8320 8321 8322	CB CC C	IRP 3 IRP 3	15 110. 15 111. 15 110. 15 111. 15 109. 15 112. 15 112. 15 113. 15 108. 16 108. 16 108. 16 106. 16 106. 16 106. 17 106. 16 106. 17 106. 17 107. 17 108. 17 108. 17 108. 17 109. 17 109. 17 104. 17 109. 17 104. 18 103. 18 102. 18 99. 18 99. 18 99. 18 99. 18 99.	672 769 376 678 654 325 705 880 321 992 990 118 877 799 653 866 786 223 995 161 941 851 154 248 524 327 775 656 537 541 415 117 970 608 613 320 464 180	52. 262 53. 741 54. 940 55. 295 54. 910 55. 295 54. 310 55. 310 57. 588 57. 588 57. 588 57. 588 57. 588 59. 772 49. 544 48. 358 47. 783 48. 026 48. 026 48. 349 44. 313 44. 367 47. 784 47. 784 47. 784 47. 784 47. 784 48. 667 47. 784 47. 784 48. 667 47. 784 48. 667 47. 784 48. 667 47. 784 48. 667 47. 784 48. 667 47. 784 48. 667 49. 342 49. 342 49. 428	20. 484 18. 968 18. 540 18. 176 17. 824 18. 113 18. 405 17. 974 17. 413 17. 704 17. 359 20. 790 20. 941 20. 872 21. 184 22. 628 23. 194 23. 408 24. 501 20. 229 20. 000 19. 666 18. 753 18. 035 16. 993 16. 321 15. 128 14. 476 14. 897 13. 401 19. 512 20. 713 18. 820 19. 476 18. 483 19. 164 18. 483 19. 164 18. 414 19. 092 18. 771 17. 771 19. 460	1.00 1.00 1.00 1.00	21. 09 21. 09 21. 09 19. 81 20. 24 17. 16 21. 12 21. 84 19. 26 22. 37 20. 90 19. 46 19. 46 19. 49 20. 73 21. 90 22. 41 19. 30 23. 49 20. 73 23. 80 20. 73 21. 57 21. 6. 73 22. 80 22. 41 23. 80 24. 95 25. 73 26. 73 27. 74 28. 81 29. 11 20. 21 20. 21 21. 22 22. 41 23. 42 24. 95 25. 57 26. 73 27. 28 28. 81 29. 21 20. 21 21. 22 22. 41 23. 42 24. 95 25. 57 26. 73 27. 28 28. 81 29. 21 20. 21 21. 22 21. 23 22. 41 23. 42 24. 95 25. 57 26. 73 27. 28 28. 81 29. 31 29. 31 20. 31 21. 59 21. 59 21. 59 22. 41 23. 42 24. 95 25. 57 26. 73 27. 59 28. 57 29. 12 20. 21 20.	B B B B B B B B B B B B B B B B B B B	CCCCCCNCCCONCCCCCCCONCCCCCNCNNCONCCCCCNCNN
ATOM ATOM ATOM ATOM	8320 8321 8322 8323	NH1 A NH2 A C A O A	ARG 3 ARG 3 ARG 3 ARG 3	18 96. 18 95. 18 102. 18 101.	464 180 085 569	50. 342 49. 428 46. 251 46. 103	17. 771 19. 460 20. 132 21. 234	1.00 1.00 1.00 1.00	13.59 12.42 15.28 15.74	B B B	N N C O
ATOM ATOM ATOM ATOM ATOM	8315 8316 8317 8318 8319	CB A CG A CD A NE A CZ A	ARG 3 ARG 3 ARG 3 ARG 3 ARG 3	18 100. 18 99. 18 98. 18 97. 18 96.	970 608 613 326 320	47. 781 47. 794 48. 660 48. 672 49. 478	18. 483 19. 164 18. 414 19. 092 18. 771	1.00 1.00 1.00 1.00 1.00	17.09 17.74 16.48 16.05 17.02	B B B B	C C N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8323 8324 8325 8326 8327 8328 8329	N I	ILE 3 ILE 3 ILE 3 ILE 3 ILE 3 ILE 3	19 102. 19 102. 19 103. 19 103. 19 101.	627 757 006 268 793	46. 103 45. 251 43. 912 42. 848 41. 519 42. 732 42. 425	21. 234 19. 440 20. 007 18. 949 19. 621 18. 036 18. 781	1.00 1 1.00 1 1.00 1 1.00 1 1.00 1	15. 27 15. 37 15. 60 17. 64 15. 37	B B B B B	O N C C C C
					-					-	=

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F I G. 4 - 1 7 1 ATOM 8330 C ILE 319 104.036 44.122 20.802 1.00 16.78 B C ATOM 8331 0 ILE 319 105.145 44.086 20.257 1.00 16.37 B 0 ATOM 8332 N GLN 320 103.850 44.367 22.092 1.00 17.82 B N ATOM 8333 CA GLN 320 104.923 44.693 23.016 1.00 18.01 B C ATOM 8334 CB GLN 320 104.293 45.341 24.248 1.00 16.84 B C ATOM 8335 CG GLN 320 104.293 45.341 24.248 1.00 16.84 B C ATOM 8335 CG GLN 320 102.833 47.250 25.048 1.00 17.06 B C ATOM 8336 CD GLN 320 102.833 47.250 25.048 1.00 17.06 B C ATOM 8337 0E1 GLN 320 103.544 47.509 26.016 1.00 18.02 B O ATOM 8338 NE2 GLN 320 101.566 47.633 24.966 1.00 16.46 B N ATOM 8339 C GLN 320 105.964 43.663 23.437 1.00 18.97 B C ATOM 8340 0 GLN 320 105.964 43.663 23.437 1.00 18.97 B C ATOM 8341 N ASN 321 106.382 42.800 22.520 1.00 19.64 B N ATOM 8341 N ASN 321 106.382 42.800 22.520 1.00 19.64 B N ATOM 8342 CA ASN 321 107.420 41.846 22.875 1.00 21.44 B C ATOM 8344 CG ASN 321 106.950 40.399 22.719 1.00 23.79 B C ATOM 8345 OD1 ASN 321 106.593 40.839 20.374 1.00 28.16 B O ATOM 8345 OD1 ASN 321 106.593 40.839 20.374 1.00 28.16 B O ATOM 8345 OD1 ASN 321 106.593 40.839 20.374 1.00 28.16 B O ATOM 8345 OD1 ASN 321 106.593 40.839 20.374 1.00 28.16 B O ATOM 8347 C ASN 321 106.593 40.839 20.374 1.00 28.16 B O ATOM 8347 C ASN 321 106.593 40.839 20.374 1.00 28.16 B O ATOM 8347 C ASN 321 106.593 40.839 20.374 1.00 28.16 B O ATOM 8347 C ASN 321 106.593 40.839 20.374 1.00 28.16 B O ATOM 8348 O ASN 321 109.533 41.228 21.940 1.00 23.87 B O ATOM 8348 O ASN 321 109.533 41.228 21.940 1.00 23.87 B O ATOM 8348 O ASN 321 109.533 41.228 21.940 1.00 23.87 B O ATOM 8348 O ASN 321 109.533 41.228 21.940 1.00 23.87 B O ATOM 8348 O ASN 321 109.533 41.228 21.940 1.00 23.87 B O ATOM 8348 O ASN 321 109.533 41.228 21.940 1.00 23.87 B O ATOM 8349 N TYR 322 108.735 43.275 21.444 1.00 20.566 B N	d)
ATOM 8331 0 ILE 319 105.145 44.086 20.257 1.00 16.37 B 0 ATOM 8332 N GLN 320 103.850 44.367 22.092 1.00 17.82 B N ATOM 8333 CA GLN 320 104.923 44.693 23.016 1.00 18.01 B C ATOM 8334 CB GLN 320 104.293 45.341 24.248 1.00 16.84 B C ATOM 8335 CG GLN 320 103.383 46.495 23.863 1.00 16.48 B C ATOM 8336 CD GLN 320 102.833 47.250 25.048 1.00 17.06 B C ATOM 8337 0E1 GLN 320 103.544 47.509 26.016 1.00 18.02 B O ATOM 8338 NE2 GLN 320 101.566 47.633 24.966 1.00 16.46 B N ATOM 8339 C GLN 320 105.964 43.663 23.437 1.00 18.97 B C ATOM 8340 O GLN 320 106.399 43.654 24.594 1.00 20.18 B O ATOM 8341 N ASN 321 106.382 42.800 22.520 1.00 19.64 B N ATOM 8342 CA ASN 321 106.382 42.800 22.520 1.00 19.64 B N ATOM 8343 CB ASN 321 106.950 40.399 22.719 1.00 23.79 B C ATOM 8344 CG ASN 321 106.409 40.085 21.332 1.00 27.68 B C ATOM 8345 OD1 ASN 321 106.593 40.839 20.374 1.00 28.16 B O ATOM 8346 ND2 ASN 321 105.745 38.934 21.255 1.00 30.91 B N ATOM 8347 C ASN 321 105.745 38.934 21.255 1.00 30.91 B N ATOM 8348 O ASN 321 109.533 41.228 21.940 1.00 23.87 B O ATOM 8348 O ASN 321 109.533 41.228 21.940 1.00 23.87 B O ATOM 8348 O ASN 321 109.533 41.228 21.940 1.00 23.87 B O ATOM 8349 N TYR 322 108.735 43.275 21.444 1.00 20.566 B N	
ATOM 8348 0 ASN 321 109.533 41.228 21.940 1.00 23.87 B O ATOM 8349 N TYR 322 108.735 43.275 21.444 1.00 20.56 B N	
ATOM 8350 CA TYR 322 109.873 43.644 20.613 1.00 18.63 B C ATOM 8351 CB TYR 322 109.605 43.208 19.178 1.00 18.95 B C	
ATOM 8353 CD1 TYR 322 111.086 44.604 17.677 1.00 21.18 B C ATOM 8354 CE1 TYR 322 112.118 44.733 16.759 1.00 22.17 B C ATOM 8355 CD2 TYR 322 111.520 42.252 17.840 1.00 20.55 B C ATOM 8356 CE2 TYR 322 112.557 42.372 16.925 1.00 21.33 B C ATOM 8357 CZ TYR 322 112.847 43.611 16.387 1.00 22.88 B C	
ATOM 8358 OH TYR 322 113.855 43.726 15.461 1.00 28.00 B O ATOM 8359 C TYR 322 110.115 45.149 20.678 1.00 18.95 B C ATOM 8360 O TYR 322 109.240 45.945 20.338 1.00 20.45 B O ATOM 8361 N SER 323 111.299 45.537 21.139 1.00 18.50 B N ATOM 8362 CA SER 323 111.657 46.946 21.233 1.00 17.89 B C ATOM 8363 CB SER 323 111.623 47.418 22.684 1.00 18.88 B C ATOM 8364 OG SER 323 112.602 46.740 23.444 1.00 21.21 B O	
ATOM 8365 C SER 323 113.057 47.131 20.677 1.00 16.99 B C ATOM 8366 O SER 323 113.851 46.190 20.657 1.00 15.79 B O ATOM 8367 N VAL 324 113.360 48.345 20.230 1.00 16.51 B N ATOM 8368 CA VAL 324 114.672 48.638 19.664 1.00 17.39 B C ATOM 8369 CB VAL 324 114.612 48.684 18.126 1.00 18.70 B C	
ATOM 8370 CG1 VAL 324 113.454 49.550 17.692 1.00 22.04 B C ATOM 8371 CG2 VAL 324 115.901 49.257 17.565 1.00 20.08 B C ATOM 8372 C VAL 324 115.201 49.970 20.151 1.00 16.54 B C ATOM 8373 O VAL 324 114.460 50.946 20.243 1.00 19.05 B O ATOM 8374 N MET 325 116.487 50.011 20.463 1.00 15.89 B N ATOM 8375 CA MET 325 117.104 51.243 20.914 1.00 16.61 B C ATOM 8376 CB MET 325 118.053 50.997 22.083 1.00 17.97 B C ATOM 8377 CG MET 325 118.682 52.280 22.597 1.00 19.56 B C ATOM 8378 SD MET 325 119.851 52.014 23.915 1.00 22.61 B S	

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(Continued) FIG. 4-172 C 8379 CE MET 325 118.765 51.442 25. 211 1.00 21.39 **ATOM** 51.875 19.782 1.00 17.82 C 8380 MET 117.895 В **ATOM** C 325 19.082 0 8381 MET 118.658 51.198 1.00 15.28 В 0 325 ATOM 117.698 53.175 19.607 1.00 18.85 B N 8382 N ASP 326 **ATOM** C 118.409 53.922 18.591 1.00 21.89 В **ATOM** 8383 CA **ASP** 326 В C 117.436 54.685 17.695 1.00 22.04 **ATOM** 8384 CB ASP 326 117.533 54.272 16.244 1.00 23.15 В **ATOM** 8385 CG **ASP** 326 8386 0D1 ASP 326 116.800 54.855 15.418 1.00 25.35 В 0 **ATOM** 118. 334 119. 299 ASP 53.366 15.922 1.00 23.67 В 0 **ATOM** 8387 0D2 326 **ASP** 54.904 19.327 1.00 24.54 В C **ATOM** 8388 C 326 0 **ASP** 326 118.896 55.494 20.335 1.00 25.63 В 0 **ATOM** 8389 **ATOM** N ILE 120.521 55.062 18.842 1.00 25.49 В N 8390 327 55.986 327 121.451 19.459 1.00 27.44 В C **ATOM** 8391 -CA ILE C 327 122.713 55.263 19.936 1.00 27.10 **ATOM** 8392 CB ILE 8393 CG2 ILE 327 123.697 56.264 20.515 1.00 27.85 В **ATOM** 54. 221 8394 CG1 ILE 327 122.321 20.984 1.00 25.49 В C **ATOM** 123, 476 53.506 1.00 27.60 C 21.594 В 8395 CD1 ILE 327 **ATOM** 121.784 57.005 18.395 1.00 29.15 В C 8396 C ILE 327 **ATOM** 327 122.357 56.673 17.357 1.00 31.19 В 0 ILE **ATOM** 8397 0 121.414 58.250 18.653 1.00 30.14 В N 8398 CYS 328 **ATOM** N 121.624 59.298 17.684 1.00 31.56 В 8399 CYS 328 ATOM CA CYS 122.624 60.356 18.084 1.00 32.64 В C 8400 C 328 ATOM CYS 328 122.525 60.972 19.153 1.00 33.03 В 0 0 **ATOM** 8401 CYS 120. 286 328 59.938 17.366 1.00 32.73 В C CB **ATOM** 8402 58.689 17.154 1.00 36.31 S SG CYS 328 118.979 В ATOM 8403 123.596 17.200 1.00 32.72 В N **ASP** 329 60.555 **ATOM** 8404 N 61.542 17.406 1.00 32.74 В C ATOM 8405 CA ASP 329 124.639 60.9751.00 34.70 В C **ATOM** 8406 CB ASP 329 125.997 16.981 ATOM 8407 CG ASP 329 126.480 59.858 17.894 1.00 36.73 В C OD1 ASP 329 127.643 59.431 17.735 1.00 38.23 В 0 8408 ATOM 8409 329 125.706 59.405 18.767 1.00 36.00 0 OD2 ASP В **ATOM** 124.320 62.781 16.588 1.00 31.70 C 8410 329 В **ATOM** C **ASP** 123.767 62.692 15.494 1.00 30.70 В 0 329 8411 0 **ASP** ATOM 124.662 17.129 1.00 31.69 В N 63.940 TYR 330 **ATOM** 8412 N В C 124.420 1.00 33.40 **ATOM** TYR 330 65.191 16.428 8413 CA C 124.376 66.354 1.00 30.81 В 8414 TYR 330 17.411 **ATOM** CB 124. 322 123. 185 C 67.693 16.728 1.00 29:75 В CG TYR 330 ATOM 8415 C 68.089 1.00 30.07 16.030 В ATOM 8416 CD1 TYR 330 Ċ 1.00 30.94 123.121 69.326 15.399 В ATOM 8417 CE1 TYR 330 16.777 1.00 30.62 C 125.407 68.568 В CD2 TYR 330 **ATOM** 8418 16.150 В C 69.814 1.00 30.16 8419 125.356 ATOM CE2 TYR 330 124.206 1.00 31.10 В 8420 330 70.186 15.465 ATOM CZ TYR 124.122 71.422 14.867 1.00 29.92 В 0 **ATOM** 8421 0H TYR 330 65.462 15.412 1.00 35.09 В C 8422 330 125.523 ATOM C TYR 15.772 1.00 36.29 8423 330 126.692 65.552 В 0 ATOM 0 TYR 14.146 1.00 37.07 В N 8424 125.149 65.600 ATOM N **ASP** 331 13.106 1.00 39.50 В C 126.123 65.886 ATOM 8425 CA **ASP** 331 11.756 1.00 39.77 C 125.611 65.391 **ATOM** 8426 CB ASP 331 126.665 65.464 10.677 1.00 40.31 **ATOM** 8427 CG ASP 331

	(Continued)
FIG. 4-173	(00227222
ATOM 8428 OD1 ASP 331 126.387 65.018 9.543 1.00 41.37 ATOM 8429 OD2 ASP 331 127.770 65.966 10.967 1.00 40.07 ATOM 8430 C ASP 331 126.355 67.395 13.062 1.00 41.19 ATOM 8431 O ASP 331 125.641 68.126 12.380 1.00 40.38 ATOM 8432 N GLU 332 127.358 67.852 13.802 1.00 44.16 ATOM 8433 CA GLU 332 127.358 67.852 13.802 1.00 44.16 ATOM 8434 CB GLU 332 127.690 69.271 13.879 1.00 47.17 ATOM 8435 CG GLU 332 129.001 69.457 14.646 1.00 48.86 ATOM 8436 CD GLU 332 129.367 70.901 14.922 1.00 51.70 ATOM 8437 OE1 GLU 332 130.451 71.028 15.979 1.00 54.56 ATOM 8438 OE2 GLU 332 130.203 70.623 17.136 1.00 55.51 ATOM 8438 OE2 GLU 332 131.552 71.528 15.658 1.00 56.11 ATOM 8439 C GLU 332 127.791 69.941 12.517 1.00 47.83 ATOM 8440 O GLU 332 127.518 71.130 12.383 1.00 48.20 ATOM 8441 N SER 333 128.179 69.175 11.505 1.00 48.69 ATOM 8442 CA SER 333 128.179 69.175 11.505 1.00 49.93	77 B O 55 B C 59 B O 66 B N 77 B C 70
ATOM 8443 CB SER 333 129. 246 68. 835 9. 327 1.00 50. 95 ATOM 8444 OG SER 333 130. 521 68. 723 9. 943 1.00 54. 48 ATOM 8445 C SER 333 126. 957 69. 809 9. 483 1.00 49. 97 ATOM 8446 O SER 333 126. 514 70. 893 9. 108 1. 00 50. 95 ATOM 8447 N SER 334 126. 302 68. 665 9. 326 1. 00 50. 21 ATOM 8448 CA SER 334 124. 993 68. 609 8. 687 1. 00 49. 04 ATOM 8449 CB SER 334 124. 582 67. 154 8. 451 1. 00 50. 46	B B C B C B C B C B N B C
ATOM 8450 0G SER 334 123.275 67.076 7.905 1.00 52.36 ATOM 8451 C SER 334 123.934 69.288 9.536 1.00 47.42 ATOM 8452 O SER 334 122.917 69.742 9.021 1.00 48.45 ATOM 8453 N GLY 335 124.177 69.353 10.840 1.00 45.55 ATOM 8454 CA GLY 335 123.219 69.965 11.738 1.00 42.54 ATOM 8455 C GLY 335 122.081 69.007 12.033 1.00 40.97	B 0 B C B 0 B N B C
ATOM 8456 0 GLY 335 121.179 69.318 12.807 1.00 40.87 ATOM 8457 N ARG 336 122.117 67.834 11.409 1.00 38.61 ATOM 8458 CA ARG 336 121.076 66.843 11.622 1.00 37.65 ATOM 8459 CB ARG 336 120.725 66.143 10.306 1.00 39.07 ATOM 8460 CG ARG 336 120.460 67.099 9.151 1.00 41.95 ATOM 8461 CD ARG 336 119.339 66.597 8.248 1.00 45.61	B O B N B C B C
ATOM 8462 NE ARG 336 118.019 67.002 8.729 1.00 48.18 ATOM 8463 CZ ARG 336 117.522 68.233 8.613 1.00 49.86 ATOM 8464 NH1 ARG 336 118.229 69.194 8.025 1.00 50.51 ATOM 8465 NH2 ARG 336 116.317 68.510 9.094 1.00 50.56 ATOM 8466 C ARG 336 121.524 65.817 12.654 1.00 35.64 ATOM 8467 O ARG 336 122.629 65.900 13.181 1.00 35.91	
ATOM 8468 N TRP 337 120.649 64.865 12.955 1.00 33.09 ATOM 8469 CA TRP 337 120.955 63.818 13.918 1.00 30.08 ATOM 8470 CB TRP 337 119.922 63.793 15.053 1.00 24.67 ATOM 8471 CG TRP 337 119.993 64.979 15.954 1.00 20.03 ATOM 8472 CD2 TRP 337 120.670 65.059 17.214 1.00 17.75 ATOM 8473 CE2 TRP 337 120.550 66.390 17.671 1.00 17.16 ATOM 8474 CE3 TRP 337 121.374 64.137 17.997 1.00 15.36 ATOM 8475 CD1 TRP 337 119.498 66.224 15.709 1.00 19.73 ATOM 8476 NE1 TRP 337 119.827 67.079 16.736 1.00 18.61	B N B C B C B C B C B C B C B C B C B C B C

		FΙ	G. 4 -	174			(Continued)
ATOM 8478 ATOM 8479 ATOM 8480 ATOM 8481 ATOM 8482 ATOM 8483 ATOM 8484 ATOM 8485 ATOM 8486 ATOM 8486 ATOM 8488 ATOM 8489 ATOM 8490 ATOM 8491 ATOM 8492 ATOM 8493 ATOM 8494 ATOM 8495 ATOM 8496 ATOM 8496 ATOM 8496 ATOM 8496 ATOM 8496 ATOM 8501 ATOM 8501 ATOM 8501 ATOM 8502 ATOM 8503 ATOM 8504 ATOM 8504 ATOM 8504 ATOM 8505 ATOM 8506 ATOM 8506 ATOM 8507 ATOM 8508 ATOM 8509 ATOM 8501 ATOM 8501 ATOM 8506 ATOM 8501 ATOM 8511	CZ2 TRP CZ3 TRP CZ3 TRP CH2 TRP C TRP O TRP N ASN CA ASN CB ASN OD1 ASN ND2 ASN OD2 ASN OD2 ASN OD2 CYS CA	337 121. 11 337 121. 93 337 120. 94 337 120. 94 337 119. 98 338 122. 07 338 123. 24 338 123. 24 338 122. 25 338 123. 29 338 121. 98 338 122. 11 339 121. 41 339 121. 45 339 121. 13 339 120. 07 339 118. 99 340 123. 21 340 123. 79 340 125. 30 340 126. 16 340 127. 50 340 126. 16 340 127. 50 340 126. 35 340 127. 50 341 122. 95 341 121. 98 341 121. 91 341 121. 93 341 121. 93 341 122. 95	0 66. 825 62. 64. 567 8 65. 900 62. 487 63 62. 167 63 61. 712 9 60. 426 60. 416 7 61. 271 62. 306 64 60. 845 65 59. 364 9 57. 104 4 60. 845 55. 296 1 55. 604 8 59. 364 9 57. 104 4 59. 294 9 57. 104 8 55. 296 1 55. 604 8 54. 491 3 55. 633 55. 257 1 52. 752 2 53. 151 1 52. 752 2 53. 151 1 50. 423 2 49. 256 2 49. 872 0 49. 872 0 49. 888 1 50. 688 1 50. 688	18. 875 19. 196 19. 622 13. 188 12. 482 13. 347 12. 691 11. 698 10. 471 10. 251 9. 669 13. 693 14. 631 13. 499 14. 385 13. 564 12. 848 14. 961 15. 160 13. 665 12. 933 13. 218 12. 609 13. 322 11. 132 13. 259 14. 418 12. 220 12. 387 11. 047 11. 175 9. 968 13. 314 14. 366 12. 913 13. 704 15. 194 16. 001 15. 561 16. 961 17. 120	1. 00 18. 08 1. 00 15. 24 1. 00 16. 71 1. 00 31. 57 1. 00 33. 23 1. 00 32. 12 1. 00 34. 88 1. 00 38. 68 1. 00 39. 82 1. 00 33. 12 1. 00 33. 48 1. 00 33. 12 1. 00 33. 60 1. 00 34. 06 1. 00 34. 06 1. 00 34. 06 1. 00 34. 61 1. 00 37. 83 1. 00 34. 61 1. 00 34. 61 1. 00 34. 61 1. 00 34. 61 1. 00 34. 61 1. 00 34. 61 1. 00 34. 61 1. 00 34. 65 1. 00 35. 87 1. 00 36. 37 1. 00 36. 37 1. 00 36. 37 1. 00 36. 74 1. 00 37. 20 1. 00 38. 15 1. 00 36. 74 1. 00 37. 20 1. 00 38. 15 1. 00 36. 74 1. 00 36. 74 1. 00 37. 20 1. 00 38. 15 1. 00 36. 76 1. 00 37. 20 1. 00 38. 15 1. 00 36. 76 1. 00 32. 62	888888888888888888888888888888888888888	CCCCONCCONCONCCOCSNCCCCCONCCCCONCCCONCC
ATOM 8507 CATOM 8508 CATOM 8509 CATOM 8510 CATOM 8511 CATOM 8512 CATOM 8513 CATOM 8514 CATOM 8515 CATOM 8516 CATOM 8516 CATOM 8517 CATOM 8518 CATOM 8519 CATOM 8520 CATOM 8521 CATOM 8522 CATOM 8523 C	CG1 VAL CG2 VAL C VAL O VAL N ALA CA ALA CB ALA C ALA O ALA N ARG CA ARG	341 121.01 341 121.53 341 122.95 341 122.51 342 124.20 342 125.13 342 126.54 342 125.09 342 125.69 343 124.41 343 124.30	2 49. 256 2 51. 391 7 50. 305 1 49. 872 0 50. 073 4 49. 283 6 49. 482 5 49. 609 8 48. 897 1 50. 688 3 51. 074 1 52. 562 3 52. 922 5 54. 396 5 54. 692 1 55. 885 6 56. 907	11. 175 9. 968 13. 314 14. 366 12. 913 13. 704 13. 178 15. 194 16. 001 15. 561 16. 961	1.00 37.20 1.00 38.15 1.00 36.74 1.00 39.77 1.00 35.94 1.00 34.75 1.00 34.74 1.00 36.76 1.00 32.52 1.00 30.81	B B B B B B B	C C O N C C C O N C

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					DIO						(Cor	tinued)
					FIG.	4 -	1 / 5					
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8526 8527 8528 8529 8530 8531 8532 8533 8534 8535 8536 8537 8538 8540 8541 8542	NE2 C O N CA CB CG CD2 ND1 CE1	ARG GLN GLN GLN GLN GLN HIS HIS HIS HIS	343 344 344 344 344 344 345 345 345 345	122. 121 5 120. 786 4 119. 944 4 118. 980 5 118. 091 4 117. 567 4 117. 905 5 120. 853 4 121. 655 4 120. 008 4 119. 977 4 120. 514 4 121. 973 4 121. 973 4 123. 062 4 122. 449 49 123. 769 49	1. 143 0. 026 9. 625 9. 238 0. 296 9. 802 8. 685 0. 632 8. 431 7. 515 8. 436 7. 753 8. 079 7. 279 9. 361 9. 337	18. 650 16. 763 17. 183 15. 974 15. 516 14. 399 14. 457 13. 378 18. 121 17. 919 19. 145 20. 085 21. 452 21. 443 21. 516 21. 270 21. 234	1. 00 28 1. 00 28 1. 00 26 1. 00 30 1. 00 31 1. 00 32 1. 00 28 1. 00 28 1. 00 28 1. 00 27 1. 00 26 1. 00 28 1. 00 27 1. 00 28 1. 00 28	. 05 . 26 . 68 . 39 . 50 . 52 . 84 . 55 . 32 . 34 . 01 . 88 . 88 . 67 . 37	B B B B B B B B B B B B B B B B B B B		
ATOM ATOM ATOM	8543 8544 8545	NE2 C O	RIH S SIH SIH	345 345 345	118.568 4	8. 086 6. 799 7. 508	21. 381 20. 215 20. 625	1.00 28 1.00 27 1.00 30	. 76	B B B	И С О	
ATOM	8546	N	ILE	346	118.396 4	5.538	19.849	1.00 26	. 83	В	N	
ATOM ATOM	8547 8548	CA CB	ILE ILE	346 346	116.977 43	4. 897 3. 842	19. 899 18. 791	1.00 25 1.00 25	56	B B	C C	
ATOM ATOM	8549 8550		ILE	$\frac{346}{346}$		3. 114 4. 517	18. 919 17. 422	1.00 26. 1.00 26.		B B	C	
ATOM	8551	CD1	ILE	346	117.180 43	3. 544	16.263	1.00 26.	42	В	C	
ATOM ATOM	8552 8553	.C 0	ILE ILE	346 346		4. 218 3. 558	21. 228 21. 776	1.00 26. 1.00 25.		B B	C 0	
ATOM	8554	N	GLU	347		1. 396	21.746	1.00 26.		В	N	
ATOM	8555	CA	GLU	347	115. 260 43	3.767	22. 994	1.00 25.	82	В	C	
ATOM	8556	CB	GLU	347		1.777	24. 134	1.00 25.		В	C	
ATOM ATOM	8557 8558	CG CD	GLU GLU	347 347		4. 118 5. 094	25. 505 26. 652	1.00 28. 1.00 29.		В	C C	
ATOM	8559		GLU	347		5. 208	26. 592	1.00 29.		B B	0	
ATOM	8560		GLU	347		1. 736	27. 628	1.00 32.		В	ő	
ATOM	8561	C	GLU	347	113.873 43	3. 172	22.799	1.00 26.	44	В	Č	
ATOM	8562	0	GLU	347		3. 889	22.495	1.00 26.		В	0	
ATOM ATOM	8563	N	MET	348		. 858	22. 957	1.00 26.		В	N	
ATOM	8564 8565	CA CB	MET MET	348 348		. 181). 767	22. 807 21. 345	1.00 27. 1.00 30.		В	C	
ATOM	8566	CG	MET	348). 132	20.660	1.00 30.		B B	C C	
ATOM	8567	SD	MET	348			21.117	1.00 42.		В	Š	
ATOM	8568	CE	MET	348			19.804	1.00 38.		B	č	
ATOM	8569	C	MET	348	112. 371 39	. 980	23. 732	1.00 26.	60	В	C	
ATOM	8570	0	MET	348			24. 247	1.00 26.		В	0	
ATOM ATOM	8571 8572	N CA	SER	349			23.950	1.00 23.		В	N	
ATOM	8572 8573	CA CB	SER SER	349 349			24. 812 25. 997	1.00 21. 1.00 20.		В	C	
ATOM	8574	0G	SER	349			26. 700	1.00 20.		B B	0 0	

										(Continu	ued)
٠.					FIC	G. 4 -	176				
ATOM	8575	C	SER	349	110.084	37. 387	24.005	1.00 21.88	В	С	
ATOM	8576	0	SER	349	109. 274	37. 739	23. 154	1.00 23.74	В	0	
ATOM	8577	N	THR	350	110. 351	36. 112	24. 264	1.00 21.76	В	N	
ATOM	8578	CA	THR	350	109. 654	35. 033	23.571	1.00 23.08	В	C	
ATOM	8579	CB	THR	350	110.603	33. 882	23. 214	1.00 22.77	В	C	
ATOM	8580	0G1		350	111.310	33. 483	24. 391	1.00 25.37	В	0	
ATOM	8581		THR	350	111.583	34. 299	22. 152	1.00 22.93	В	C	
ATOM	8582	C	THR	350	108. 561	34. 453	24.475	1.00 22.93	В	C	
ATOM	8583	0	THR	350	107. 732	33.650	24.035	1.00 20.70	В	0	
ATOM	8584	N	THR	351	108. 564	34.871	25.737	1.00 22.30	В	N	
ATOM	8585	CA	THR	351	107.601	34. 366	26. 703	1.00 22.35	В	C	
ATOM	8586	CB	THR	351	108. 332	33. 796	27. 932	1.00 23.36	В	C	
ATOM	8587	0G1		351	108. 989	34. 859	28. 635	1.00 25.67	В	0	
ATOM	8588		THR	351	109. 378	32. 781	27. 493	1.00 22.26	В	C	
ATOM	8589	C	THR	351	106.575	35. 392	27. 171	1.00 21.07	В	C	
ATOM	8590	0	THR	351	105.562	35. 031	27.760	1.00 20.87	В	0	
ATOM	8591	N	GLY	352	106.839	36.668	26. 918	1.00 19.83	В	N	
ATOM	8592	CA	GLY	352	105.894	37. 692	27. 325	1.00 19.36	В	C	
ATOM	8593	C	GLY	352	106.182	39. 027	26.672	1.00 18.63	В	C	
ATOM	8594	0	GLY	352	106.633	39.076	25.531	1.00 20.78	В	0	
ATOM	8595	N	TRP TRP	353	105.913	40.109	27. 397	1.00 17.51	В	N	
ATOM ATOM	8596 8597	CA CB	TRP	353 353	106. 156 105. 195	41.464 42.451	26. 907 27. 587	1.00 15.30	В	C	
ATOM	8598	CG	TRP	353	105. 195	42. 451	29. 084	1.00 13.08 1.00 9.17	В	C	
ATOM	8599		TRP	353	103. 103	41.387	29. 877	1.00 9.17	B B	C	
ATOM	8600		TRP	353	104. 739	41. 684	31. 233	1.00 8.17	В	C C	
ATOM	8601		TRP	353	103. 671	40. 288	29. 574	1.00 10.72	В	č	
ATOM	8602		TRP	353	105. 798	43. 195	29.966	1.00 11.19	В	C	
ATOM	8603	NE1		353	105. 546	42. 791	31.265	1.00 10.10	В	N	
ATOM	8604		TRP	353	104. 217	40. 921	32. 281	1.00 10.66	B	Ĉ	
ATOM	8605	CZ3		353	103. 149	39. 524	30. 625	1.00 10.40	B	č	
ATOM	8606	CH2		353	103. 426	39. 848	31.958	1.00 9.81	B	č	
ATOM	8607	C	TRP	353	107. 594	41.796	27. 264	1.00 15.80	B	č	
ATOM	8608	0	TRP	353	108. 247	40.999	27.931	1.00 16.59	B	Ö	
ATOM	8609	N	VAL	354	108.092	42.946	26.819	1.00 13.84	В	N	
ATOM	8610	CA	VAL	354	109.464	43. 338	27.140	1.00 13.65	В	C	
ATOM	8611	CB	VAL	354	110. 135	44.096	25.960	1.00 16.06	В	C	
ATOM	8612		VAL	354	111.506	44.646	26.400	1.00 12.56	В	C	
ATOM	8613		VAL	354	110. 284	43. 163	24. 751	1.00 12.49	В	С	
ATOM	8614	C	VAL	354	109. 486	44. 248	28.368	1.00 13.83	В	C	
ATOM	8615	0	VAL	354	108. 716	45. 197	28.456	1.00 13.93	В	0	
ATOM	8616	N	GLY	355	110. 373	43. 957	29. 313	1.00 14.87	В	N	
MOTA	8617	CA	GLY	355	110.467	44. 769	30. 519	1.00 16.09	В	C	
ATOM	8618	C	GLY	355	109. 333	44. 554	31.513	1.00 16.34	В	C	
ATOM	8619	0	GLY	355	108. 347	43. 877	31. 206	1.00 18.25	В	0	
ATOM	8620	N	ARG	356	109. 456	45. 126	32. 706	1.00 15.16	В	N	
ATOM	8621	CA	ARG	356	108. 404	44. 953	33. 701	1.00 16.32	В	C	
ATOM	8622	CB	ARG	356	108. 856	45. 494	35.066	1.00 14.18	В	C	
ATOM	8623	CG	ARG	356	110.001	44. 668	35.667	1.00 13.44	В	C	

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(Continued) FIG. 4-177 37.151 C 8624 CD ARG 110.169 44.878 1.00 14.42 ATOM 356 111.546 45.211 37.511 1.00 18.65 N 8625 NE ATOM ARG 356 В 37.935 C CZARG 44.341 1.00 20.17 ATOM 8626 356 112.457 В 38.065 112.156 43.055 1.00 22.71 N **ATOM** NH1 ARG 356 В 8627 NH2 ARG 113.674 44.765 38. 242 1.00 18.93 N **ATOM** 8628 356 В 107. 111 33. 209 33. 066 45.607 1.00 16.01 C ATOM 8629 C ARG 356 В 356 106.100 44.924 1.00 16.29 0 ATOM 8630 0 ARG В 32.945 357 107.140 46.911 1.00 15.89 N ATOM 8631 N PHE В ATOM ATOM 105.967 32.402 8632 PHE 357 47.603 1.00 16.40 C CA В 105. 418 104. 753 33.366 C 8633 PHE 357 48.660 1.00 11.21 CB В 34.573 48.083 1.00 C ATOM 8634 CG PHE 357 8.48 В ATOM 8635 CD1 PHE 357 105.467 47.878 35.748 1.00 5.58 В C 103.407 **ATOM** 8636 CD2 PHE 357 47.711 34.531 1.00 8.57 В C 104.846 ATOM 8637 PHE 357 47.309 36.867 1.00 5.98 В CE1 102.777 35.648 C ATOM 8638 CE2 PHE 357 47.136 1.00 4.59 В 103.498 46.937 36.812 C ATOM 8639 CZPHE 357 1.00 3.60 В 106. 344 105. 476 ATOM ATOM 8640 C PHE 48.259 31.076 1.00 18.69 C 357 B 48.638 30.287 1.00 21.57 8641 0 PHE В 0 357 48.377 30.840 **ATOM** 8642 N ARG 107.648 1.00 19.12 В N 358 48.953 **ATOM** 8643 CA ARG 358 108.188 29.612 1.00 19.47 В C 107.826 50.439 29.499 1.00 19.02 ATOM 8644 CB ARG 358 В C ATOM CG ARG 358 . 108. 451 51.346 30.559 1.00 19.99 8645 B 1.00 22.48 **ATOM** 8646 CD ARG 358 108.074 52.820 30.338 В C 108.633 53.708 ATOM 8647 NE ARG 358 31.362 1.00 24.20 В N 109. 204 109. 304 ATOM CZ54.890 31.117 1.00 24.69 8648 ARG 358 В C ATOM 8649 ARG 55.358 1.00 21.14 NH1 358 29.875 В N ATOM 8650 ARG 109.696 55.603 1.00 24.33 NH2 358 32.121 В N 109. 707 110. 302 ATOM 48.784 29.646 1.00 20.57 В 8651 C **ARG** 358 C 1.00 22.16 В ATOM 8652 ARG 358 48.704 30.722 0 0 ATOM 8653 PR₀ 359 110.355 48.723 28.473 1.00 20.23 В N N 109.783 ATOM 8654 CD **PRO** 359 48.894 27.124 1.00 20.61 В C 111.816 - 112.137 ATOM ATOM PR₀ 8655 CA 359 48.564 28.411 1.00 20.48 В C 8656 CB PR₀ 359 48.916 26.959 1.00 19.85 В C ATOM CG PR₀ 110.919 26.229 C 8657 359 48.431 1.00 21.21 В 112. 527 112. 221 ATOM C 49.494 29.402 C 8658 PR₀ 359 1.00 20.23 В 0 **PRO** 29.465 **ATOM** 8659 359 50.683 1.00 22.01 В 0 **ATOM** 113.474 8660 N SER 360 48.953 30.163 1.00 19.33 В N 114. 212 115. 122 49.725 **ATOM** 8661 CA SER 360 31.160 1.00 18.75 В C ATOM 48.806 В 8662 CB SER 31.968 1.00 20.74 360 C ATOM 8663 116.163 В 0G SER 360 48.286 31.149 1.00 26.03 0 115.060 1.00 18.77 ATOM 8664 C SER 360 50.841 30.560 В C 115. 410 115. 394 1.00 17.99 **ATOM** 8665 0 50.806 29.382 В SER 360 0 **ATOM GLU** 31.393 B 8666 N 361 51.824 1.00 18.96 N ATOM 8667 GLU 116.199 52.970 30.978 CA 361 1.00 18.11 В C ATOM 8668 CB **GLU** 115.982 54.159 31.919 C 361 1.00 16.34 В GLU Ċ ATOM CG 8669 361 116.654 54.007 33.269 1.00 21.67 В ATOM 8670 CD GLU 361 115.743 53.431 34.342 1.00 27.42 В C ATOM 8671 OE1 GLU 361 115.067 52.408 34.091 1.00 28.62 В 0

54.009 **SUBSTITUTE SHEET (RULE 26)**

35. 453

1.00 31.11

В

115.710

OE2 GLU

361

ATOM

8672

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							(Continued)
				F I G. 4 - 1	178		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
ATOM	8673	C GI	LU 361	117.674 52.595	31.007 1.00) 16.97 B	С
ATOM	8674	0 GI) 16.23 B	
ATOM	8675	N PI) 16.09 B	
ATOM	8676	CD PI) 13.66 B	C
ATOM	8677	CA PI) 15.32 B	С
ATOM	8678	CB PI) 13.19 B	
ATOM	8679	CG PI) 12.78 B	
ATOM	8680	C PI) 16.34 B	
ATOM	8681	0 PI) 17. 05 B	
ATOM	8682	N H) 17. 21 B	
ATOM	8683	CA H) 18.58 B	C
ATOM	8684	CB H) 18. 05 B	C
ATOM	8685 8686	CG HI) 19. 33 B	C
ATOM ATOM	8687	ND1 H) 19.36 B) 18.40 B	C
ATOM	8688	CE1 H) 19.50 B	N C
ATOM	8689	NE2 H) 22.85 B	N N
ATOM	8690	C H) 19. 40 B	Č
ATOM	8691	0 H) 19. 73 B	ŏ
ATOM	8692	N PH) 19. 14 B	Ň
ATOM	8693	CA PI) 19. 25 B	Ċ
ATOM	8694	CB PI) 17. 71 B	č
ATOM	8695	CG PF				15.99 B	Ċ
ATOM	8696	CD1 PF	E 364		27.826 1.00	12.83 B	C
MOTA	8697	CD2 PF	E 364	124. 989 55. 770 2	26.656 1.00	12.86 B	C
ATOM	8698	CE1 PF			26.781 1.00	8. 09 B	C
ATOM	8699	CE2 PF				10.87 B	C
ATOM	8700	CZ PF			25.679 1.00		C
ATOM	8701	C PF				18. 72 B	C
ATOM	8702	0 PF				17. 88 B	0
ATOM	8703	N TH				18. 23 B	N
ATOM	8704	CA TH				19. 73 B	C
ATOM	8705	CB TH				17. 73 B	C
ATOM	8706	OG1 TH				22.16 B	0
ATOM	8707	CG2 TH				13.36 B	C
ATOM	8708	C TH				20.48 B	C
MOTA	8709 8710	0 TH				20. 68 B 22. 60 B	0 N
ATOM ATOM	8711	N LE					N C
ATOM	8712	CB LE				25. 75 B 29. 32 B	C C
ATOM	8713	CG LE				34. 01 B	C
ATOM	8714	CD1 LE				33.57 B	C
ATOM	8715	CD2 LE				34. 78 B	Č
ATOM	8716	C LE				26. 20 B	Č
ATOM	8717	0 LE				26.53 B	Ŏ
ATOM	8718	N AS				24. 26 B	Ň
ATOM	8719	CA AS				23. 63 B	Ċ
ATOM	8720	CB AS				23.47 B	č
ATOM	8721	CG AS				25. 27 B	C

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				FIG. 4-179	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8722 8723 8724 8725 8726 8727 8728 8729 8730 8731 8732 8733 8734 8735 8736 8737	OD1 ASP OD2 ASP C ASP O ASP N GLY CA GLY C GLY N ASN CA ASN CB ASN CG ASN OD1 ASN ND2 ASN C ASN O ASN	367 367 367 368 368 369 369 369 369 369 369	FIG. 4 - 179 132.158 56.515 27.507 1.00 24.35 B 134.311 56.634 27.935 1.00 25.99 B 130.810 58.990 26.767 1.00 22.76 B 130.848 59.261 25.568 1.00 24.31 B 129.795 58.348 27.330 1.00 20.91 B 128.646 57.950 26.547 1.00 18.80 B 128.912 56.843 25.550 1.00 19.81 B 128.059 56.563 24.700 1.00 19.55 B 130.073 56.198 25.643 1.00 19.20 B 130.398 55.117 24.706 1.00 19.60 B 131.907 54.986 24.526 1.00 19.65 B 132.519 56.217 23.921 1.00 21.94 B 132.005 56.757 22.945 1.00 25.32 B 133.628 56.671 24.489 1.00 23.16 B 129.828 53.760 25.090 1.00 18.53 B 129.770 52.861 24.258 1.00 18.17	(Continued) 0 0 C 0 N C C 0 N C C 0 N C C 0 N C C 0 O 0 N C 0 0 0 0 0
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8738 8739 8740 8741 8742 8743 8744 8745 8746 8747 8748 8749 8750	N SER CA SER CB SER OG SER O SER N PHE CA PHE CB PHE CC PHE CD1 PHE CD2 PHE CD1 PHE	370 370 370 370 370 371 371 371 371 371 371	129. 420 53. 608 26. 346 1. 00 18. 61 B 128. 847 52. 347 26. 812 1. 00 19. 50 B 129. 934 51. 447 27. 430 1. 00 20. 45 B 130. 577 52. 057 28. 538 1. 00 22. 81 B 127. 746 52. 621 27. 829 1. 00 18. 95 B 127. 562 53. 759 28. 261 1. 00 19. 22 B 127. 009 51. 583 28. 209 1. 00 18. 63 B 125. 931 51. 763 29. 168 1. 00 18. 66 B 124. 762 52. 516 28. 512 1. 00 19. 79 B 124. 088 51. 756 27. 398 1. 00 16. 47 B 124. 532 51. 874 26. 093 1. 00 15. 63 B 122. 991 50. 940 27. 660 1. 00 17. 78 B 123. 893 51. 198 25. 059 1. 00 18. 99 B	N C C O C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8751 8752 8753 8754 8755 8756 8757 8758 8759 8760 8761	CE2 PHE CZ PHE C PHE O PHE N TYR CA TYR CB TYR CG TYR CD1 TYR CD2 TYR CD2 TYR CE2 TYR	371 371 371 372 372 372 372 372 372 372 372	122. 340 50. 255 26. 631 1. 00 18. 61 B 122. 792 50. 386 25. 327 1. 00 18. 10 B 125. 402 50. 473 29. 784 1. 00 18. 78 B 125. 506 49. 392 29. 197 1. 00 17. 45 B 124. 814 50. 614 30. 970 1. 00 19. 00 B 124. 240 49. 491 31. 703 1. 00 18. 59 B 124. 697 49. 527 33. 159 1. 00 17. 86 B 126. 199 49. 500 33. 290 1. 00 17. 83 B 126. 951 50. 676 33. 201 1. 00 19. 52 B 128. 339 50. 651 33. 257 1. 00 18. 29 B 126. 878 48. 296 33. 441 1. 00 17. 45 B 128. 266 48. 257 33. 498 1. 00 18. 99 B	C C O N C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8763 8764 8765 8766 8767 8768 8769 8770	CZ TYR OH TYR C TYR O TYR N LYS CA LYS CB LYS CG LYS	372 372 372 372 373 373 373 373	128. 991 49. 434 33. 405 1. 00 18. 83 B 130. 364 49. 387 33. 454 1. 00 19. 89 B 122. 727 49. 558 31. 620 1. 00 18. 38 B 122. 143 50. 632 31. 717 1. 00 20. 19 B 122. 096 48. 406 31. 436 1. 00 19. 10 B 120. 647 48. 340 31. 299 1. 00 18. 51 B 120. 285 48. 376 29. 809 1. 00 17. 90 B 118. 809 48. 581 29. 485 1. 00 21. 01 B	C O C O N C C C

										(Continued)
				٠,	FI	G. 4	- 180			(Continued)
ATOM	8771	CD	LYS	373	118. 59	3 48.627	27.969	1.00 21.40	В	С
ATOM	8772	CE	LYS	373	117.24			1.00 21.67	В	C
ATOM	8773	NZ	LYS	373	116.05			1.00 21.98	В	N
ATOM	8774	C	LYS	373	120.12			1.00 18.77	В	C
ATOM	8775	0	LYS	373	120.69			1.00 18.48	В	0
ATOM	8776	N	ILE	374	119.05			1.00 17.06	В	Ŋ
ATOM	8777	CA	ILE	374	118. 47			1.00 15.88	В	C
ATOM	8778	CB	ILE	374	117. 55			1.00 14.58	В	C
ATOM	8779		ILE	374	116.95			1.00 12.18	В	C
ATOM	8780		ILE	374	118.34			1.00 15.07	В	C
ATOM	8781		ILE	374	117.51			1.00 13.03	В	C
ATOM	8782	C	ILE	374	117.61			1.00 16.94	В	C
ATOM	8783	0	ILE	374	116.64			1.00 17.41	B B	O N
ATOM	8784	N	ILE	375	117.97			1.00 18.50 1.00 19.71	В	C
ATOM	8785	CA CB	ILE ILE	375 375	117. 17 117. 84			1.00 19.71	В	C
ATOM ATOM	8786 8787		ILE	375	118.12			1.00 19.02	В	Č
ATOM	8788		ILE	375	119.12			1.00 21.23	В	č
ATOM	8789		ILE	375	119.82			1.00 23.06	B	č
ATOM	8790	C	ILE	375	116.98			1.00 20.44	В	č
ATOM	8791	ŏ	ILE	375	117.73			1.00 20.03	B	Ŏ
ATOM	8792	Ň	SER	376	115.96			1.00 21.14	В	N
ATOM	8793	CA	SER	376	115.70			1.00 21.95	В	C
ATOM	8794	CB	SER	376	114.34			1.00 21.55	В	C
ATOM	8795	0G	SER	376	114.02	6 38.054	31.539	1.00 25.40	В	0
ATOM	8796	C	SER	376	116.80	8 38.899	30.936	1.00 23.06	В	C
ATOM	8797	0	SER	376	117. 23			1.00 24.16	В	0
ATOM	8798	N	ASN	377	117. 28			1.00 24.67	В	N
ATOM	8799	CA	ASN	377	118. 35			1.00 25.07	В	C
ATOM	8800	CB	ASN	377	119.43			1.00 23.49	В	Č
ATOM	8801	CG	ASN	377	119.01			1.00 23.86	В	Ç.
ATOM	8802		ASN	377	117. 95			1.00 23.70	В	0
ATOM	8803		ASN	377	119.84			1.00 20.11	В	N
ATOM	8804	C	ASN	377	117.89			1.00 26.79	В	C
ATOM	8805	0	ASN	377	116.70			1.00 28.58	В	0
ATOM	8806	N	GLU	378	118.86			1.00 29.97	В	N C
ATOM	8807	CA CB	GLU GLU	378	118.60 119.91			1.00 33.15 1.00 37.08	B B	C C
ATOM ATOM	8808 8809	CG	GLU	378 378	120. 69			1.00 37.08	В	C
ATOM	8810	CD	GLU	378	120. 03			1.00 45.76	В	C
ATOM	8811		GLU	378	121.00			1.00 40.50	В	0
ATOM ATOM	8812		GLU	378	122. 90			1.00 47.91	В	0
ATOM	8813	C	GLU	378	117.58			1.00 33.63	В	č
ATOM	8814	ŏ	GLU	378	116.68			1.00 35.16	В	ŏ
ATOM	8815	N	GLU	379	117.74			1.00 32.70	В	Ň
ATOM	8816	CA	GLU	379	116.83			1.00 30.44	В	Ċ
ATOM	8817	CB	GLU	379	117.54			1.00 34.46	B	Č
ATOM	8818	CG	GLU	379	117. 84			1.00 39.45	В	Č
ATOM	8819	CD	GLU	379	116.57			1.00 43.32	В	C

					(Continued)
				FIG. 4-181	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8820 8821 8822 8823 8824 8825 8826 8827 8830 8831 8832 8833 8834 8835 8836 8837 8838 8839 8840 8841 8842 8843	OE1 GLU OE2 GLU O GLU N GLY C GLY O GLY O GLY N TYR CA TYR CA TYR CB TYR CCI T	379 379 379 380 380 380 381 381 381 381 381 381 381 381 381 381	FIG. 4 - 181 115.800	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8843 8844 8845 8846 8847 8848 8850 8851 8852 8853 8854 8855 8856 8857 8858 8859 8860 8861 8862 8863 8864	CD ARG NE ARG CZ ARG NH1 ARG NH2 ARG C ARG O ARG N HIS CA HIS CB HIS CCB ILE CCB ILE CCB ILE	382 382 382 382 382 382 383 383 383 383	113. 948 41. 478 34. 606 1.00 15. 55 B 112. 581 42. 001 34. 993 1.00 17. 88 B 111. 576 41. 337 34. 170 1.00 19. 19 B 111. 438 41. 515 32. 859 1.00 21. 25 B 112. 230 42. 357 32. 203 1.00 18. 86 B 110. 534 40. 810 32. 190 1.00 23. 20 B 117. 438 41. 172 36. 140 1.00 12. 33 B 117. 497 41. 376 37. 349 1.00 9. 83 B 118. 474 41. 303 35. 323 1.00 11. 97 B 119. 778 41. 711 35. 789 1.00 12. 81 B 120. 377 39. 496 36. 813 1.00 12. 29 B 120. 377 39. 496 36. 813 1.00 13. 83 B 119. 726 38. 313 36. 721 1.00 12. 69 B 120. 670 39. 675 38. 148 1.00 16. 23 B 119. 635 37. 803 37. 993 1.00 14. 04 B 120. 351 <	C N N C O N C C C C N C O N C C C C C C
ATOM ATOM ATOM ATOM	8865 8866 8867 8868	CG1 ILE CD1 ILE C ILE O ILE	384 384 384 384	122. 071	C C C C

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							(Continued)
]	FIG. 4	183			
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8918 CG ASP 8919 OD1 ASP 8920 OD2 ASP 8921 C ASP 8922 O ASP 8923 N LYS 8924 CA LYS 8925 CB LYS 8926 CG LYS 8927 CD LYS 8927 CD LYS 8928 CE LYS 8929 NZ LYS 8930 C LYS 8931 O LYS 8932 N LYS	390 130 390 120 390 13 390 120 390 120 391 120 391 120 391 130 391 130 391 130 391 130 391 130 391 130 391 130	0. 576 51. 416 9. 879 51. 713 1. 349 52. 227 8. 887 48. 106 8. 589 47. 557 9. 081 47. 427 8. 967 45. 977 9. 981 45. 409 1. 416 45. 724 2. 428 45. 397 3. 816 45. 911 4. 822 45. 719 7. 550 45. 535 5. 857 46. 191 7. 125 44. 419	17. 816 1 16. 819 1 18. 372 1 18. 675 1 17. 619 1 19. 798 1 19. 826 1 20. 818 1 20. 407 1 21. 494 1 21. 112 1 22. 192 1 20. 163 1 20. 942 1	1. 00 49. 16 1. 00 50. 13 1. 00 50. 30 1. 00 44. 93 1. 00 47. 19 1. 00 45. 32 1. 00 45. 91 1. 00 47. 86 1. 00 51. 34 1. 00 55. 03 1. 00 55. 62 1. 00 56. 68 1. 00 45. 76 1. 00 46. 28 1. 00 44. 97	B B B B B B B B B B B B B B B B B B B	C O O C O N C C C C C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8933 CA LYS 8934 CB LYS 8935 CG LYS 8936 CD LYS 8937 CE LYS 8938 NZ LYS 8939 C LYS 8940 O LYS 8941 N ASP	392 125 392 125 392 124 392 124 392 123 392 124 392 125 392 124 393 126	5. 772 43. 916 5. 218 43. 382 4. 750 44. 494 4. 282 43. 970 3. 533 45. 057 4. 298 46. 338 5. 529 42. 895 4. 386 42. 512 5. 579 42. 446	19. 782 1 18. 458 1 17. 529 1 16. 186 1 15. 436 1 15. 419 1 20. 886 1 21. 134 1	1. 00 45. 02 1. 00 46. 84 1. 00 49. 00 1. 00 50. 10 1. 00 51. 49 1. 00 52. 49 1. 00 43. 84 1. 00 44. 15 1. 00 41. 92	B B B B B B B	C C C C C C C C N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8942 CA ASP 8943 CB ASP 8944 CG ASP 8945 OD1 ASP 8946 OD2 ASP 8947 C ASP 8948 O ASP 8949 N CYS	393 127 393 125 393 125 393 128 393 126 393 127 394 125	3. 381 41. 489 4. 289 40. 268 4. 022 39. 509 3. 39. 350 39. 062 4. 685 42. 158 42. 588 42. 588 678 42. 252	22. 470 1 21. 194 1 20. 824 1 20. 569 1 23. 953 1 24. 188 1 24. 816 1	. 00 40. 21 . 00 41. 22 . 00 41. 43 . 00 40. 27 . 00 43. 49 . 00 38. 67 . 00 39. 07 . 00 35. 47	B B B B B B B	C C C O O C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8950 CA CYS 8951 C CYS 8952 O CYS 8953 CB CYS 8954 SG CYS 8955 N THR 8956 CA THR 8957 CB THR 8958 OG1 THR	394 126 394 126 394 124 394 123 395 126 395 127 395 128	882 42.870 374 41.796 248 40.608 586 43.491 354 42.328 938 42.215 462 41.279 964 41.493 627 41.265	27. 069 1 26. 787 1 26. 639 1 27. 301 1 28. 193 1 29. 171 1 29. 358 1	. 00 32. 02 . 00 29. 62 . 00 29. 41 . 00 31. 92 . 00 33. 67 . 00 26. 53 . 00 23. 76 . 00 23. 30 . 00 25. 56	B B B B B B B	C C C S N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8959 CG2 THR 8960 C THR 8961 O THR 8962 N PHE 8963 CA PHE 8964 CB PHE 8965 CG PHE 8966 CD1 PHE	395 129 395 126 395 126 396 126 396 125 396 124 396 123	. 518 40. 542	30. 397 1. 30. 519 1. 31. 035 1. 31. 095 1. 32. 396 1. 32. 652 1. 31. 918 1.	. 00 22. 48 . 00 22. 20 . 00 23. 25 . 00 19. 02 . 00 18. 94 . 00 17. 62 . 00 19. 32	B B B B B B B	C C O N C C C

											(Cont	inued)
					FIC	3.4-	184				,	
ATOM	8967	CD2	PHE	396	123. 265	38. 378	30. 837	1.00 19	9. 67	В	С	
ATOM	8968	CE1		396	121. 267	40.157	31.593	1.00 21		В	C	
ATOM	8969	CE2		396	122.062	38.411	30.130	1.00 20	0. 02	В	С	
ATOM	8970	CZ	PHE	396	121.057	39. 303	30. 507	1.00 22		В	C	
ATOM	8971	C	PHE	396	126.712	40.596	33. 488	1.00 19		В	C	
ATOM	8972	0	PHE	396	127. 703	39.866	33.516	1.00 21		В	0	
ATOM	8973	N	ILE	397	126. 511	41.559	34. 380	1.00 17		В	N	
ATOM	8974	CA	ILE	397	127. 454	41.774	35. 460	1.00 14		В	Č	
ATOM	8975	CB	ILE	397	127. 819	43. 240	35. 566	1.00 14		В	C	
ATOM	8976	CG2		397	128. 181	43. 762	34. 192	1.00 14		В	C	
ATOM	8977	CG1		397	126. 644	44.036	36. 135	1.00 13		В	C	
ATOM	8978	CD1		397	126. 993	45. 472	36. 449	1.00 11		В	C	
ATOM	8979	Ç	ITE	397	126. 885	41. 287	36. 791	1.00 16		В	C	
ATOM	8980	0	ILE	397	127. 543	41.376	37. 833	1.00 18		В	0	
ATOM	8981	N	THR	398	125.651	40. 790	36.753	1.00 15		В	N	
ATOM	8982	CA	THR	398	125.000	40. 241	37. 937	1.00 14		В	C	
ATOM	8983	CB	THR	398	124. 049	41.255	38.652	1.00 14		В	C	
ATOM	8984	OG1		398	122. 968	41.627	37. 784	1.00 13 1.00 13		B B	0 C	
ATOM	8985	CG2	THR	398	124.812	42. 476 39. 040	39. 083 37. 490	1.00 15		В	·C	
ATOM	8986	C		398 398	124. 185 123. 805	38. 942	36. 323	1.00 15		В	Õ	
ATOM	8987 8988	O N	THR LYS	399	123. 915	38. 127	38. 416	1.00 17		В	N	
ATOM ATOM	8989		LYS	399	123. 313	36. 935	38. 094	1.00 18		В	Č	
ATOM	8990	CB	LYS	399	124. 026	35.960	37. 314	1.00 20		В	Č	
ATOM	8991		LYS	399	125. 322	35.630	38. 023	1.00 24		В	Č	
ATOM	8992	CD	LYS	399	125. 970	34. 380	37. 458	1.00 29		В	Č	
ATOM	8993	CE	LYS	399	127. 055	33. 860	38. 402	1.00 32		B	č	
ATOM	8994	NZ	LYS	399	128. 082	34. 904	38. 703	1.00 34		B	Ň	
ATOM	8995	C	LYS	399	122.616	36. 259	39. 354	1.00 17		B	Ċ	
ATOM	8996	ŏ	LYS	399	123.041	36. 571	40.465	1.00 18		B	ŏ	
ATOM	8997	Ň	GLY	400	121.684	35. 331	39. 181	1.00 16		B	Ň	
ATOM	8998	CA	GLY	400	121. 131	34.640	40. 327	1.00 17		B	Ċ	
ATOM	8999	C	GLY	400	119.616	34.629	40.320	1.00 19		В	Č	
ATOM	9000	0	GLY	400	118.979	35.360	39.551	1.00 22		В	0	
ATOM	9001	N	THR	401	119.028	33. 797	41.172	1.00 18		В	N	
ATOM	9002	CA	THR	401	117. 582	33.708	41.227	1.00 17	. 93	В	C	
ATOM	9003	CB	THR	401	117. 125	32.323	41.700	1.00 17	. 98	В	C	
ATOM	9004	0G1	THR	401	117.653	32.056	43.004	1.00 20	0. 05	В	0	
ATOM	9005	CG2		401	117. 607	31. 267	40.730	1.00 13		В	C	
ATOM	9006	C	THR	401	117. 013	34. 785	42. 125	1.00 16		В	C	
ATOM	9007	0	THR	401	116. 478	34. 519	43. 192	1.00 18		В	0	
ATOM	9008	N	TRP	402	117. 155	36.013	41.659	1.00 16		В	N	
ATOM	9009	CA	TRP	402	116.671	37. 199	42. 335	1.00 14		В	C	
ATOM	9010	CB	TRP	402	117. 528	37. 503	43. 561	1.00 16		В	C	
ATOM	9011	CG	TRP	402	119.001	37. 502	43. 296	1.00 16		В	C	
ATOM	9012	CD2		402	119. 793	38. 614	42.861	1.00 17		В	C	
ATOM	9013	CE2		402	121. 131	38. 164	42. 771	1.00 18		В	C	
ATOM	9014	CE3		402	119.504	39. 948	42.542	1.00 18		В	C	
ATOM	9015	CD1	TKP	402	119.859	36. 453	43.440	1.00 16	. ZU	В	С	

					FIG	. 1 -	186			(Continued)
					riG	• 4 -	100			
ATOM	9065	C	GLU	408	121.687	55.094	40.888	1.00 19.22	В	C
ATOM	9066	0	GLU	408	121.468	56.306	40. 924	1.00 21.06	В	0
ATOM	9067	N	ALA	409	122. 899	54. 589	40. 678 40. 473	1.00 18.36	В	N C
ATOM	9068 9069	CA CB	ALA ALA	409 409	124. 048 124. 533	55. 463 56. 012	40.473	1.00 17.37 1.00 16.78	B B	C C
ATOM ATOM	9070	CB	ALA	409	125. 189	54. 756	39. 755	1.00 10.16	В	C
ATOM	9071	Ö	ALA	409	125. 323	53. 536	39. 834	1.00 15.91	В	Ö
ATOM	9072	Ň	LEU	410	126.009	55. 545	39.062	1.00 17.35	B	Ň
ATOM	9073	CA	LEU	410	127.140	55.034	38. 311	1.00 17.53	В	C
ATOM	9074	CB	LEU	410	126.722	54.817	36.857	1.00 16.60	В	C
ATOM	9075	CG	LEU	410	127. 767	54. 292	35. 862	1.00 18.12	В	C
ATOM	9076		LEU	410	128. 278	52.914	36. 302	1.00 16.12	В	C
ATOM	9077		LEU	410	127. 144	54. 224	34. 467	1.00 14.82	В	C
MOTA	9078	C	LEU	410		55.969	38. 356	1.00 18.72	В	C
ATOM	9079	0	LEU	410		57.175	38. 190	1.00 20.28 1.00 18.37	В	0 N
ATOM ATOM	9080 9081	N CA	THR THR	411 411		55. 396 56. 142	38. 589 38. 617	1.00 18.37	B B	N C
ATOM	9082	CB	THR	411		56. 286	40.060	1.00 13.21	В	Č
ATOM	9083	0G1		411		55.024	40.514	1.00 17.72	В	Ö
ATOM	9084		THR	411		56.764	41.012	1.00 17.11	В	č
ATOM	9085	C	THR	411		55. 293	37. 784	1.00 20.67	B	Č
ATOM	9086	0	THR	411		54. 200	37. 357	1.00 23.60	В	0
ATOM	9087	N	SER	412		55. 772	37.543	1.00 21.07	В	N
ATOM	9088	CA	SER	412		54. 988	36. 753	1.00 21.08	В	C
ATOM	9089	CB	SER	412		55. 827	36. 365	1.00 18.37	В	C
ATOM	9090	0G	SER	412		56.086	37. 496	1.00 21.11	В	0
ATOM	9091	C	SER	412		53. 778	37. 548	1.00 22.07	В	C
ATOM	9092 9093	O N	SER ASP	412	134.961	52. 843	36.995	1.00 23.13	В	0
ATOM ATOM	9094	CA	ASP	413 413		53. 790 52. 677	38. 850 39. 673	1.00 22.17 1.00 22.98	B B	N C
ATOM	9095	CB	ASP	413		53. 198	40. 895	1.00 22.98	В	C
ATOM	9096	CG	ASP	413		53. 697	40. 548	1.00 28.45	В	Č
ATOM	9097		ASP	413		54. 395	41.389	1.00 31.52	В	0 .
ATOM	9098		ASP	413		53. 385	39. 444	1.00 29.95	\tilde{B}	ŏ
ATOM	9099	C	ASP	413		51.777	40.123	1.00 22.23	В	Č
ATOM	9100	0	ASP	413	133.624	50. 565	40. 248	1.00 22.67	В	0
ATOM	9101	N	TYR	414		52. 362	40. 351	1.00 21.41	В	N
ATOM	9102	CA	TYR	414		51.575	40.819	1.00 18.45	В	C
ATOM	9103	CB	TYR	414		51. 708	42. 329	1.00 15.46	В	Č
ATOM	9104	CG	TYR	414		51.071	43. 131	1.00 14.79	В	C
ATOM ATOM	9105 9106		TYR	414		49.699	43. 357	1.00 14.59	В	C
ATOM	9107		TYR TYR	414 414		49.120	44. 159 43. 718	1.00 16.87	В	C
ATOM	9108		TYR	414		51.850 51.282	43. 718	1.00 14.91 1.00 16.48	B B	C C
ATOM	9109	CZ	TYR	414		49. 921	44. 733	1.00 16.46	В	C
ATOM	9110	OH	TYR	414		49. 369	45. 541	1.00 10.20	В	Ö
ATOM	9111	C	TYR	414		51.898	40. 214	1.00 17.91	В	č
ATOM	9112	0	TYR	414		52. 990	39. 693	1.00 17.06	B	Ö
ATOM	9113	N	LEU	415		50. 917	40. 323	1.00 16.46	В	N

				FIG. 4-188	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9163 9164 9165 9166 9167 9168 9170 9171 9172 9173 9174 9175 9176 9177 9180 9181 9182 9183 9184 9185 9186	OD1 ASN ND2 ASN C ASN O ASN N GLU CA GLU CB GLU CB GLU OE1 GLU OE2 GLU O GLU N TYR CA TYR CA TYR CB TYR CG TYR CCI TYR	420 420 420 421 421 421 421 421 421 422 422 422 422	F I G. 4 - 188 115. 220	0 N C C C C C C C C C C C C C C C C C C
ATOM	9185 9186 9187 9188 9189 9190 9191 9192 9193 9194 9195 9196 9197 9198 9199 9200 9201 9202 9203 9204 9205 9206	OH TYR C TYR O TYR N LYS CA LYS CB LYS CG LYS CD LYS CE LYS NZ LYS C LYS O LYS N GLY CA GLY CA GLY CA GLY CA GLY CA MET CA MET CB MET CC MET CE MET	422 422 423 423 423 423 423 423 423 424 424	121. 267 40. 376 56. 637 1. 00 28. 92 B 118. 401 38. 600 51. 114 1. 00 20. 84 B 117. 187 38. 779 51. 012 1. 00 22. 40 B 118. 933 37. 546 51. 732 1. 00 21. 52 B 118. 130 36. 486 52. 340 1. 00 21. 53 B 117. 436 36. 995 53. 608 1. 00 22. 83 B 118. 393 37. 278 54. 751 1. 00 25. 85 B 117. 677 37. 707 56. 020 1. 00 27. 71 B 118. 692 38. 082 57. 098 1. 00 31. 46 B 118. 052 38. 548 58. 367 1. 00 31. 96 B 117. 097 35. 906 51. 378 1. 00 21. 44 B 116. 114 35. 293 51. 797 1. 00 22. 16 B 117. 331 36. 106 50. 086 1. 00 20. 50 B 116. 430 35. 595 49. 070 1. 00 <td>0 C O N C C C O N C C C C C C C C C C C C</td>	0 C O N C C C O N C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM	9208 9209 9210	C MET O MET N PRO CD PRO CA PRO	425 425 426 426 426	112. 908 38. 604 48. 871 1. 00 16. 75 B 113. 405 39. 725 48. 819 1. 00 17. 33 B 111. 968 38. 206 47. 999 1. 00 16. 64 B 111. 173 36. 969 48. 017 1. 00 17. 29 B 111. 530 39. 089 46. 910 1. 00 15. 29 B	C O N C C

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					(Continued)	,
				FIG. 4-189	(commucu)	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9212 9213 9214 9215 9216 9217 9220 9221 9222 9223 9224 9225 9226 9227 9228 9229 9230	CB PRO CG PRO C PRO O PRO N GLY CA GLY O GLY N GLY C GLY O GLY N ARG CA ARG CA ARG CB ARG CC ARG CC ARG CC ARG CC ARG	426 426 426 427 427 427 428 428 428 429 429 429 429 429 429	110. 523 38. 233 46. 140 1. 00 15. 30 110. 816 36. 823 46. 561 1. 00 15. 73 110. 901 40. 379 47. 416 1. 00 15. 48 110. 913 41. 402 46. 727 1. 00 15. 90 110. 362 40. 321 48. 630 1. 00 14. 46 109. 718 41. 480 49. 217 1. 00 13. 34 110. 649 42. 449 49. 919 1. 00 13. 11 110. 184 43. 462 50. 452 1. 00 14. 26 111. 947 42. 144 49. 942 1. 00 9. 68 112. 902 43. 036 50. 577 1. 00 8. 65 113. 735 43. 771 49. 538 1. 00 10. 35 113. 778 43. 363 48. 377 1. 00 10. 03 114. 406 44. 844 49. 946 1. 00 11. 09 115. 224 45. 630 49. 023 1. 00 12. 98 114. 349 46. 667 48. 314 1. 00 14. 68 113. 580 46. 084 47. 144 1. 00 18. 69 111. 590 46. 279 45. 699 1. 00 19. 88	(Continued) B C B C B C B O B N B C B C B C B C B C B C B C B C B C B C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9229 9230 9231 9232 9233 9234 9235 9236 9237 9238 9240 9241 9242 9243 9244 9245 9246	NE ARG CZ ARG NH1 ARG NH2 ARG C ARG O ARG N ASN CA ASN CB ASN CG ASN OD1 ASN ND2 ASN C ASN O ASN N LEU CA LEU CB LEU CG LEU	429 429 429 429 429 430 430 430 430 431 431 431	111. 590 46. 279 45. 699 1. 00 19. 88 111. 184 45. 008 45. 769 1. 00 21. 09 111. 535 44. 227 46. 791 1. 00 17. 36 110. 390 44. 520 44. 825 1. 00 20. 65 116. 420 46. 328 49. 678 1. 00 13. 64 116. 291 46. 983 50. 707 1. 00 13. 96 117. 584 46. 198 49. 056 1. 00 12. 81 118. 784 46. 812 49. 585 1. 00 13. 48 119. 605 45. 767 50. 344 1. 00 11. 94 118. 985 45. 411 51. 677 1. 00 12. 47 119. 104 46. 167 52. 652 1. 00 11. 56 118. 293 44. 277 51. 727 1. 00 7. 39 119. 530 47. 189 47. 335 1. 00 14. 26 119. 530 47. 189 47. 335 1. 00 16. 18 121. 425 49. 107 48. 135 1. 00 17. 01 121. 709 50. 496	B N B C B N B C B C B C B C B C B C B C B C B C B C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9247 9248 9249 9250 9251 9252 9253 9254 9255 9256 9257 9258 9259 9260	CD1 LEU CD2 LEU C LEU O LEU N TYR CA TYR CB TYR CG TYR CD1 TYR CD2 TYR CD2 TYR CE2 TYR CZ TYR OH TYR	431 431 432 432 432 432 432 432 432 432 432 432	122. 501 51. 399 46. 528 1. 00 17. 30 B 122. 998 52. 651 48. 667 1. 00 14. 93 B 122. 729 48. 338 48. 022 1. 00 17. 39 B 123. 367 48. 018 49. 028 1. 00 19. 06 B 123. 112 48. 038 46. 789 1. 00 17. 62 B 124. 344 47. 317 46. 511 1. 00 18. 05 B 124. 061 45. 978 45. 826 1. 00 17. 24 B 123. 334 44. 944 46. 654 1. 00 18. 80 B 121. 962 45. 034 46. 883 1. 00 19. 62 B 121. 289 44. 049 47. 601 1. 00 19. 23 B 124. 015 43. 843 47. 169 1. 00 17. 63 B 123. 360 42. 862 47. 882 1. 00 18. 49 B 121. 996 42. 968 48. 099 1. 00 20. 13 B 121. 358 41. 994 48. 834 1. 00 21. 75 B	C C C C C C C C C C C C C C C C C C C	

					(Continued)
				FIG. 4-190	
ATOM	9261	C TY			B C
ATOM	9262	0 TY			B 0
ATOM	9263	N L			B N
ATOM ATOM	9264 9265	CA LY			B C B C
ATOM	9266	CG LY			B C B C
ATOM	9267	CD LY			B C
ATOM	9268	CE LY		and the second s	B Č
ATOM	9269	NZ LY			B N
ATOM	9270	C LY	rs 433	128. 269 47. 343 44. 058 1. 00 13. 68 I	ВС
ATOM	9271	0 LY		128.654 46.454 44.820 1.00 11.44 I	
ATOM	9272	N II		128. 564 47. 364 42. 767 1. 00 13. 85	
ATOM	9273	CA II		129. 411 - 46. 331 42. 191 1. 00 15. 56	
ATOM ATOM	9274 9275	CB II CG2 II		128. 645 45. 504 41. 124 1. 00 14. 45 I	
ATOM	9276	CG2 II		128. 054 46. 429 40. 061 1. 00 11. 95 129. 580 44. 458 40. 518 1. 00 14. 14	
ATOM	9277	CD1 II		129.580 44.458 40.518 1.00 14.14 F 128.978 43.676 39.379 1.00 14.42 F	
ATOM	9278	C IL		130. 646 46. 973 41. 573 1. 00 16. 13	
ATOM	9279	0 IL		130. 554 48. 003 40. 915 1. 00 17. 71	
ATOM	9280	N GL		131.804 46.374 41.809 1.00 18.33 E	
ATOM	9281	CA GL		133.045 46.907 41.263 1.00 20.88 E	
ATOM	9282	CB GL		134. 253 46. 264 41. 956 1. 00 21. 76	
ATOM	9283	CG GL		135. 490 47. 145 41. 958 1. 00 24. 28 E	
ATOM	9284	CD GL		136. 715 46. 461 42. 547 1. 00 25. 69 B	
ATOM ATOM	9285 9286	OE1 GL NE2 GL		136.763 46.154 43.741 1.00 26.08 B 137.713 46.220 41.705 1.00 24.68 B	
ATOM	9287	C GL		137.713 46.220 41.705 1.00 24.68 B 133.068 46.617 39.767 1.00 20.60 B	
ATOM	9288	0 GL		132.969 45.465 39.348 1.00 20.57 B	
ATOM	9289	N LE		133. 200 47. 668 38. 965 1. 00 21. 54 B	
ATOM	9290	CA LE		133.197 47.527 37.513 1.00 23.39 B	
ATOM	9291	CB LE		133.050 48.905 36.880 1.00 21.46 B	
ATOM	9292	CG LE		131.785 49.596 37.386 1.00 19.80 B	
ATOM	9293	CD1 LE		131.748 51.035 36.920 1.00 19.31 B	C
ATOM	9294	CD2 LE		130. 572 48. 831 36. 895 1. 00 18. 85 B	
ATOM	9295	C LE		134. 391 46. 790 36. 908 1. 00 25. 55 B	
ATOM ATOM	9296 9297	O LE N SE		134. 294 46. 242 35. 810 1. 00 27. 46 B	-
ATOM	9298	CA SE		135. 517 46. 775 37. 613 1. 00 26. 98 B 136. 690 46. 069 37. 119 1. 00 26. 89 B	
ATOM	9299	CB SE		136.690 46.069 37.119 1.00 26.89 B 137.967 46.683 37.689 1.00 26.26 B	
ATOM	9300	OG SE		137.940 46.694 39.102 1.00 31.19 B	
ATOM	9301	C SE		136. 593 44. 597 37. 507 1. 00 27. 29 B	
ATOM	9302	0 SE		137.152 43.736 36.832 1.00 29.17 B	
ATOM	9303	N AS	P 438	135.882 44.310 38.595 1.00 26.66 B	
ATOM	9304	CA ASI		135. 704 42. 930 39. 049 1. 00 26. 32 B	C
ATOM	9305	CB AS		136. 702 42. 588 40. 151 1. 00 28. 65 B	C
ATOM	9306	CG AS		136. 622 41. 135 40. 571 1. 00 30. 81 B	
ATOM ATOM	9307 9308	OD2 AS		135. 517 40. 557 40. 495 1. 00 32. 19 B	
ATOM	9309	OD2 ASI		137. 659 40. 575 40. 990 1. 00 33. 46 B 134. 286 42. 691 39. 572 1. 00 24. 90 B	
UIOM	5005	o no	400	134. 286 42. 691 39. 572 1. 00 24. 90 B	С

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ATOM 9310 O ASP 438 133.959 43.060 40.700 1.00 22.15 B O ATOM 9311 CA TYR 439 132.083 41.780 39.123 1.00 23.79 B N ATOM 9312 CA TYR 439 132.083 41.780 39.123 1.00 23.74 B C ATOM 9313 CB TYR 439 131.301 41.243 37.924 1.00 22.94 B C ATOM 9314 CG TYR 439 131.301 41.243 37.924 1.00 22.94 B C ATOM 9315 CDI TYR 439 131.420 43.514 36.814 1.00 22.94 B C ATOM 9315 CDI TYR 439 131.420 43.514 36.814 1.00 22.19 B C ATOM 9316 CDI TYR 439 131.420 43.514 36.814 1.00 22.19 B C ATOM 9317 CDI TYR 439 131.322 41.572 35.416 1.00 22.08 B C ATOM 9317 CDI TYR 439 131.322 41.572 35.416 1.00 22.08 B C ATOM 9317 CDI TYR 439 131.342 44.329 35.416 1.00 22.08 B C ATOM 9318 CEITR 439 131.405 43.753 34.430 1.00 21.92 B C ATOM 9320 DH TYR 439 131.405 43.753 34.430 1.00 21.92 B C ATOM 9320 DH TYR 439 131.405 43.753 34.430 1.00 21.92 B C ATOM 9320 DH TYR 439 131.405 43.753 34.430 1.00 21.92 B C ATOM 9320 DH TYR 439 131.405 43.753 34.430 1.00 21.92 B C ATOM 9320 DH TYR 439 131.405 43.753 34.430 1.00 21.92 B C ATOM 9320 DH TYR 439 131.405 43.753 34.430 1.00 21.92 B C ATOM 9320 DH TYR 439 131.405 43.753 34.430 1.00 21.92 B C ATOM 9320 CD TYR 439 131.405 43.753 40.823 1.00 22.11 B C ATOM 9320 CD TYR 439 131.405 43.753 40.823 1.00 22.11 B N ATOM 9321 C TYR 439 130.882 40.823 40.823 40.294 1.00 24.24 B O ATOM 9320 CD TYR 439 131.410 44.552 33.314 1.00 24.24 B O ATOM 9320 CD TYR 439 131.410 44.552 33.314 1.00 22.70 B O ATOM 9326 C THR 440 132.953 40.030 40.584 1.00 22.11 B N ATOM 9327 CEITR 440 132.953 40.304 41.693 1.00 25.27 B O ATOM 9326 C GI THR 440 132.2583 39.994 41.699 1.00 23.35 B C ATOM 9326 C GI THR 440 134.102 38.196 41.806 1.00 23.70 B C ATOM 9330 N LYS 441 133.201 41.407 41.806 1.00 22.70 B O ATOM 9331 C A LYS 441 133.201 41.407 41.806 1.00 22.79 B C ATOM 9333 C A LYS 441 133.805 44.243 1.00 22.20 B C C ATOM 9333 C A LYS 441 133.805 44.243 1.00 22.80 B N ATOM 9334 C A VAL 442 13.686 42.741 44.375 1.00 22.86 B N ATOM 9334 C A VAL 442 13.866 64.274 43.89 1.00 22.86 B N ATOM 9334 C A VAL 442 13.886 44.284 50.00 44.889 1.00 22.86 B N ATOM 934						(Continued)
ATOM 9311 N TYR 439 133.461 42.046 38.753 1.00 23.79 B N ATOM 9312 CA TYR 439 132.083 41.780 39.123 1.00 23.74 B C ATOM 9313 CB TYR 439 131.301 41.243 37.924 1.00 22.94 B C ATOM 9316 CEI TYR 439 131.301 41.243 37.924 1.00 22.91 B C ATOM 9316 CEI TYR 439 131.420 43.514 36.814 1.00 22.44 B C ATOM 9316 CEI TYR 439 131.322 41.572 35.416 1.00 22.19 B C ATOM 9316 CEI TYR 439 131.322 41.572 35.416 1.00 22.19 B C ATOM 9316 CEI TYR 439 131.324 42.379 34.285 1.00 21.13 B C ATOM 9319 CZ TYR 439 131.324 42.379 34.285 1.00 21.13 B C ATOM 9320 OH TYR 439 131.348 42.379 34.285 1.00 21.13 B C ATOM 9321 C TYR 439 131.400 43.553 1.00 22.19 B C ATOM 9321 C TYR 439 131.400 43.553 1.00 21.92 B C ATOM 9321 C TYR 439 131.400 44.552 33.314 1.00 24.24 B O ATOM 9322 O TYR 439 131.400 45.552 33.314 1.00 24.24 B O ATOM 9322 O TYR 439 131.400 44.552 33.314 1.00 24.24 B O ATOM 9322 O TYR 439 130.882 40.801 40.933 1.00 25.27 B O ATOM 9325 CB THR 440 132.858 39.994 41.699 1.00 24.38 B C ATOM 9325 CB THR 440 132.858 39.994 41.699 1.00 23.35 B C ATOM 9326 OGI THR 440 134.102 38.196 41.699 1.00 23.35 B C ATOM 9326 CB THR 440 134.102 38.196 41.699 1.00 23.35 B C ATOM 9326 CB THR 440 134.102 38.196 41.699 1.00 23.35 B C ATOM 9328 C THR 440 134.102 38.196 41.806 1.00 23.70 B C ATOM 9328 C THR 440 134.271 238.552 40.002 2.279 B C ATOM 9331 CA LYS 441 133.200 41.087 43.099 1.00 22.29 B C ATOM 9331 CA LYS 441 133.200 41.087 43.099 1.00 22.86 B N ATOM 9331 CA LYS 441 133.291 41.905 44.243 11.00 24.29 B C ATOM 9331 CA LYS 441 133.291 41.905 44.243 11.00 22.99 B C ATOM 9331 CA LYS 441 133.891 42.792 44.878 1.00 34.36 B C ATOM 9334 CD LYS 441 133.893 41.804 44.875 1.00 22.89 B C ATOM 9336 NZ LYS 441 138.893 41.804 44.878 1.00 34.36 B C ATOM 9336 NZ LYS 441 138.893 41.804 44.878 1.00 21.84 B O ATOM 9336 NZ LYS 441 138.893 41.804 41.905 44.243 1.00 22.99 B C ATOM 9336 NZ LYS 441 138.893 41.804 42.299 40.293 1.00 22.89 B C ATOM 9336 NZ LYS 441 138.893 41.804 42.299 42.299 40.333 1.00 22.89 B C ATOM 9344 C AVAL 442 129.624 42.994 42.994 43.299 1.00 17.59 B C					FIG. 4-191	(0011011111000)
ATOM 9329 0 THR 440 132.169 39.328 43.987 1.00 21.81 B 0 ATOM 9330 N LYS 441 133.200 41.087 43.039 1.00 22.86 B N ATOM 9331 CA LYS 441 133.23 41.905 44.243 1.00 22.90 B C ATOM 9332 CB LYS 441 134.396 42.741 44.375 1.00 25.86 B C ATOM 9333 CG LYS 441 135.620 41.878 44.682 1.00 30.20 B C ATOM 9334 CD LYS 441 136.871 42.702 44.878 1.00 34.36 B C ATOM 9335 CE LYS 441 138.053 41.804 45.201 1.00 37.32 B C ATOM 9336 NZ LYS 441 139.319 42.577 45.346 1.00 40.04 B N ATOM 9337 C LYS 441 131.881 42.794 44.329 1.00 21.89 B C ATOM 9338 0 LYS 441 131.881 42.794 44.329 1.00 21.89 B C ATOM 9339 N VAL 442 130.880 42.289 45.039 1.00 19.62 B N ATOM 9340 CA VAL 442 129.624 42.984 45.242 1.00 17.69 B C ATOM 9341 CB VAL 442 128.458 42.093 44.799 1.00 17.33 B C ATOM 9342 CG1 VAL 442 128.586 41.792 43.306 1.00 11.20 B C ATOM 9345 CG2 VAL 442 128.586 41.792 43.306 1.00 11.20 B C ATOM 9345 C VAL 442 129.502 43.299 46.733 1.00 20.40 B C ATOM 9346 N THR 443 129.129 44.528 47.676 1.00 22.17 B C ATOM 9348 CB THR 443 129.129 44.528 47.066 1.00 22.17 B C ATOM 9349 CG1 THR 443 129.129 44.528 47.066 1.00 22.17 B C ATOM 9349 CG1 THR 443 129.129 44.528 47.066 1.00 22.17 B C ATOM 9349 CG1 THR 443 129.129 44.528 47.066 1.00 22.17 B C ATOM 9350 CG2 THR 443 129.129 44.528 47.066 1.00 22.17 B C ATOM 9350 CG2 THR 443 129.129 44.528 47.066 1.00 22.17 B C ATOM 9350 CG2 THR 443 129.129 44.528 47.066 1.00 22.17 B C ATOM 9350 CG2 THR 443 129.129 44.528 47.066 1.00 22.17 B C ATOM 9351 C THR 443 129.129 44.528 47.066 1.00 22.17 B C ATOM 9351 C THR 443 129.129 44.528 47.066 1.00 22.17 B C ATOM 9351 C THR 443 129.129 44.528 47.066 1.00 22.17 B C ATOM 9351 C THR 443 129.129 44.528 47.066 1.00 22.17 B C ATOM 9351 C THR 443 129.129 44.528 47.066 1.00 22.17 B C ATOM 9355 C CYS 444 126.948 44.835 49.754 1.00 21.88 B N ATOM 9351 C THR 443 129.015 44.835 49.754 1.00 21.88 B N ATOM 9351 C THR 443 129.05 44.835 49.754 1.00 21.88 B N ATOM 9355 C CYS 444 126.948 44.835 49.754 1.00 21.88 B N ATOM 9355 C CYS 444 126.948 44.835 49.754 1.00 24.50 B C ATOM 9355 C CYS 444 126.94	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9311 9312 9313 9314 9315 9316 9317 9318 9320 9321 9322 9323 9324 9325 9326 9327 9328	N CA CB CCD1 CCD2 CCE2 CZ OH CC ON CCA CCB CCB CCB CCB CCB CCB CCB CCB CCB	TYR 43 TYR 44 THR 44 THR 44 THR 44	8 133.959 43.060 40.700 1.00 22.15 B 9 133.461 42.046 38.753 1.00 23.79 B 9 132.083 41.780 39.123 1.00 23.74 B 9 131.301 41.243 37.924 1.00 22.94 B 9 131.357 42.125 36.698 1.00 22.91 B 9 131.420 43.514 36.814 1.00 22.44 B 9 131.422 43.514 36.814 1.00 22.19 B 9 131.322 41.572 35.416 1.00 22.08 B 9 131.348 42.379 34.285 1.00 21.13 B 131.405 43.753 34.430 1.00 21.92 B 9 131.410 44.552 33.314 1.00 24.24 B 9 131.928 40.823 40.294 1.00 24.38 B 130.882 40.801 40.933 1.00 25.27	0 N C C C C C C C C O C O N C C C O C
ATOM 9334 CD LYS 441 136.871 42.702 44.878 1.00 34.36 B C ATOM 9335 CE LYS 441 138.053 41.804 45.201 1.00 37.32 B C ATOM 9336 NZ LYS 441 139.319 42.577 45.346 1.00 40.04 B N ATOM 9337 C LYS 441 131.881 42.794 44.329 1.00 21.89 B C ATOM 9338 O LYS 441 131.881 42.794 44.329 1.00 21.89 B C ATOM 9339 N VAL 442 130.880 42.289 45.039 1.00 11.84 B O ATOM 9340 CA VAL 442 130.880 42.289 45.039 1.00 17.69 B C ATOM 9341 CB VAL 442 129.624 42.984 45.242 1.00 17.69 B C ATOM 9342 CG1 VAL 442 128.458 42.093 44.799 1.00 17.33 B C ATOM 9343 CG2 VAL 442 127.123 42.770 45.119 1.00 15.79 B C ATOM 9345 CVAL 442 129.502 43.299 46.733 1.00 20.40 B C ATOM 9345 O VAL 442 129.502 43.299 46.733 1.00 20.40 B C ATOM 9346 N THR 443 129.129 44.528 47.066 1.00 22.84 B O ATOM 9347 CA THR 443 129.129 44.528 47.066 1.00 22.17 B C ATOM 9348 CB THR 443 129.129 44.528 47.066 1.00 22.17 B C ATOM 9348 CB THR 443 130.040 46.035 48.801 1.00 22.17 B C ATOM 9349 OG1 THR 443 131.370 45.566 48.546 1.00 28.90 B O ATOM 9350 CG2 THR 443 129.923 46.422 50.255 1.00 22.91 B C ATOM 9351 C THR 443 127.641 45.475 48.819 1.00 23.06 B C ATOM 9351 C THR 443 127.641 45.475 48.819 1.00 23.06 B C ATOM 9353 N CYS 444 126.948 44.835 49.754 1.00 26.29 B O ATOM 9357 CB CYS 444 126.968 46.411 51.941 1.00 19.89 B O ATOM 9357 CB CYS 444 125.963 46.516 51.115 1.00 20.79 B C ATOM 9357 CB CYS 444 125.963 46.516 51.115 1.00 20.79 B C ATOM 9357 CB CYS 444 125.963 46.516 51.115 1.00 20.79 B C ATOM 9357 CB CYS 444 125.963 46.516 51.115 1.00 20.79 B C ATOM 9357 CB CYS 444 125.963 46.516 51.115 1.00 20.79 B C ATOM 9357 CB CYS 444 125.963 46.516 51.115 1.00 20.79 B C ATOM 9357 CB CYS 444 125.963 46.516 51.115 1.00 20.79 B C ATOM 9357 CB CYS 444 125.963 46.516 51.115 1.00 20.79 B C ATOM 9357 CB CYS 444 125.963 46.516 51.115 1.00 20.79 B C ATOM 9357 CB CYS 444 126.866 46.411 51.941 1.00 19.89 B O ATOM 9357 CB CYS 444 124.801 44.328 50.878 1.00 24.50 B C	ATOM ATOM ATOM ATOM	9329 9330 9331 9332	O I N I CA I CB I	THR 44 LYS 44 LYS 44 LYS 44	132.169 39.328 43.987 1.00 21.81 B 133.200 41.087 43.039 1.00 22.86 B 133.123 41.905 44.243 1.00 22.90 B 134.396 42.741 44.375 1.00 25.86 B	O N C
ATOM 9339 N VAL 442 130.880 42.289 45.039 1.00 19.62 B N ATOM 9340 CA VAL 442 129.624 42.984 45.242 1.00 17.69 B C ATOM 9341 CB VAL 442 128.458 42.093 44.799 1.00 17.33 B C ATOM 9342 CG1 VAL 442 127.123 42.770 45.119 1.00 15.79 B C ATOM 9343 CG2 VAL 442 128.586 41.792 43.306 1.00 11.20 B C ATOM 9344 C VAL 442 129.502 43.299 46.733 1.00 20.40 B C ATOM 9345 O VAL 442 129.742 42.437 47.572 1.00 22.84 B O ATOM 9346 N THR 443 129.129 44.528 47.066 1.00 20.64 B N ATOM 9347 CA THR 443 129.015 44.927 48.461 1.00 22.17 B C ATOM 9348 CB THR 443 130.040 46.035 48.801 1.00 24.13 B C ATOM 9349 OG1 THR 443 131.370 45.566 48.546 1.00 28.90 B O ATOM 9350 CG2 THR 443 129.923 46.442 50.255 1.00 22.91 B C ATOM 9351 C THR 443 127.641 45.475 48.819 1.00 23.06 B C ATOM 9353 N CYS 444 126.948 44.835 49.754 1.00 21.88 B N ATOM 9355 C CYS 444 126.948 44.835 49.754 1.00 21.88 B N ATOM 9357 CB CYS 444 125.656 45.368 50.163 1.00 20.79 B C ATOM 9357 CB CYS 444 126.866 46.411 51.941 1.00 19.89 B O ATOM 9357 CB CYS 444 126.866 46.411 51.941 1.00 19.89 B O ATOM 9357 CB CYS 444 126.866 46.411 51.941 1.00 19.89 B O ATOM 9357 CB CYS 444 126.866 46.411 51.941 1.00 19.89 B O	ATOM ATOM ATOM ATOM	9334 9335 9336 9337	CD I CE I NZ I C I	LYS 44 LYS 44 LYS 44 LYS 44	136. 871	C C N
ATOM 9344 C VAL 442 129.502 43.299 46.733 1.00 20.40 B C ATOM 9345 0 VAL 442 129.742 42.437 47.572 1.00 22.84 B O ATOM 9346 N THR 443 129.129 44.528 47.066 1.00 20.64 B N ATOM 9347 CA THR 443 129.015 44.927 48.461 1.00 22.17 B C ATOM 9348 CB THR 443 130.040 46.035 48.801 1.00 24.13 B C ATOM 9349 OG1 THR 443 131.370 45.566 48.546 1.00 28.90 B O ATOM 9350 CG2 THR 443 129.923 46.442 50.255 1.00 22.91 B C ATOM 9351 C THR 443 127.641 45.475 48.819 1.00 23.06 B C ATOM 9352 O THR 443 127.210 46.483 48.254 1.00 26.29 B O ATOM 9353 N CYS 444 126.948 44.835 49.754 1.00 21.88 B N ATOM 9355 C CYS 444 125.656 45.368 50.163 1.00 22.22 B C ATOM 9355 C CYS 444 125.963 46.516 51.115 1.00 20.79 B C ATOM 9357 CB CYS 444 126.866 46.411 51.941 1.00 19.89 B O ATOM 9357 CB CYS 444 124.801 44.328 50.878 1.00 24.50 B C	ATOM ATOM ATOM ATOM	9339 9340 9341 9342	N V CA V CB V CG1 V	VAL 449 VAL 449 VAL 449 VAL 449	130.880 42.289 45.039 1.00 19.62 B 129.624 42.984 45.242 1.00 17.69 B 128.458 42.093 44.799 1.00 17.33 B 127.123 42.770 45.119 1.00 15.79 B	N C C C
ATOM 9349 OG1 THR 443 131.370 45.566 48.546 1.00 28.90 B O ATOM 9350 CG2 THR 443 129.923 46.442 50.255 1.00 22.91 B C ATOM 9351 C THR 443 127.641 45.475 48.819 1.00 23.06 B C ATOM 9352 O THR 443 127.210 46.483 48.254 1.00 26.29 B O ATOM 9353 N CYS 444 126.948 44.835 49.754 1.00 21.88 B N ATOM 9354 CA CYS 444 125.656 45.368 50.163 1.00 22.22 B C ATOM 9355 C CYS 444 125.963 46.516 51.115 1.00 20.79 B C ATOM 9356 O CYS 444 126.866 46.411 51.941 1.00 19.89 B O ATOM 9357 CB CYS 444 124.801 44.328 50.878 1.00 24.50 B C	ATOM ATOM ATOM ATOM	9344 9345 9346 9347	C V O V N T CA T	/AL 442 /AL 442 THR 443 THR 443	129.502 43.299 46.733 1.00 20.40 B 129.742 42.437 47.572 1.00 22.84 B 129.129 44.528 47.066 1.00 20.64 B 129.015 44.927 48.461 1.00 22.17 B	C O N C
ATOM 9354 CA CYS 444 125.656 45.368 50.163 1.00 22.22 B C ATOM 9355 C CYS 444 125.963 46.516 51.115 1.00 20.79 B C ATOM 9356 O CYS 444 126.866 46.411 51.941 1.00 19.89 B O ATOM 9357 CB CYS 444 124.801 44.328 50.878 1.00 24.50 B C	ATOM ATOM ATOM ATOM	9349 9350 9351 9352	OG1 T CG2 T C T O T	THR 443 THR 443 THR 443 THR 443	131. 370 45. 566 48. 546 1. 00 28. 90	0 C C 0
	ATOM ATOM ATOM ATOM	9354 (9355 (9356 (9357 (CA C C C O C CB C	CYS 444 CYS 444 CYS 444 CYS 444	125. 656 45. 368 50. 163 1. 00 22. 22 B 125. 963 46. 516 51. 115 1. 00 20. 79 B 126. 866 46. 411 51. 941 1. 00 19. 89 B 124. 801 44. 328 50. 878 1. 00 24. 50 B	C C O C

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						(Continued)
					FIG. 4-193	(Continued)
мтом	9408	CC	DDΩ	4E 1	120. 209 43. 253 61. 290 1. 00 21. 78 B	C
ATOM ATOM	9409	CG C	PRO PRO	451 451	120. 209 43. 253 61. 290 1. 00 21. 78 B 117. 035 43. 774 60. 509 1. 00 23. 49 B	C C
ATOM	9410	Õ	PRO	451	116.125 43.392 59.774 1.00 25.06 B	Ö
ATOM	9411	N	GLU	452	116.850 44.003 61.800 1.00 24.25 B	N
ATOM	9412	CA	GLU	452	115. 539 43. 793 62. 394 1. 00 26. 56 B	Č
ATOM	9413	CB	GLU	452	115. 650 43. 767 63. 920 1. 00 32. 21 B	č
ATOM	9414	ČĞ	GLU	452	116.621 42.720 64.455 1.00 39.54 B	č
ATOM	9415	CD	GLU	452	116.666 42.675 65.976 1.00 44.38 B	Č
ATOM	9416		GLU	452	117. 355 41. 782 66. 521 1. 00 47. 19 B	0
ATOM	9417	0E2	GLU	452	116.019 43.529 66.627 1.00 46.89 B	0
· ATOM	9418	C	GLU	452	114.543 44.867 61.968 1.00 25.59 B	C
ATOM	9419	0	GLU	452	113. 374 44. 582 61. 733 1. 00 27. 44 B	0
ATOM	9420	N	ARG	453	115.010 46.101 61.848 1.00 23.36 B	N
ATOM	9421	CA	ARG	453	114. 132 47. 198 61. 478 1. 00 21. 67 B	C
ATOM	9422	CB	ARG	453	114. 539 48. 463 62. 234 1. 00 21. 94 B	C
ATOM	9423	CG	ARG	453	113. 714 49. 685 61. 872 1. 00 20. 24 B	C
ATOM	9424	CD	ARG	453	114.165 50.878 62.662 1.00 17.23 · B	C
ATOM ATOM	9425 9426	NE CZ	ARG ARG	453	113. 364 52. 058 62. 375 1. 00 16. 99 B 113. 582 53. 245 62. 927 1. 00 17. 21 B	N
ATOM	9427	NH1		453 453	113. 582 53. 245 62. 927 1. 00 17. 21 B 114. 579 53. 391 63. 791 1. 00 17. 27 B	C N
ATOM	9428		ARG	453	112. 813 54. 280 62. 619 1. 00 14. 66 B	N N
ATOM	9429	C	ARG	453	114.077 47.527 59.994 1.00 21.78 B	C
ATOM	9430	ŏ	ARG	453	113.024 47.910 59.477 1.00 20.58 B	0
ATOM	9431	Ň	CYS	454	115. 206 47. 368 59. 312 1. 00 21. 64 B	N
ATOM	9432	CA	CYS	454	115. 293 47. 715 57. 903 1. 00 19. 87 B	Ċ
ATOM	9433	C	CYS	454	115.598 46.616 56.896 1.00 19.70 B	Č
ATOM	9434	0	CYS	454	116. 698 46. 074 56. 865 1. 00 21. 81 B	0
ATOM	9435	CB	CYS	454	116. 295 48. 847 57. 770 1. 00 19. 47 B	C
ATOM	9436	SG	CYS	454	115.666 50.300 58.650 1.00 18.98 B	S
ATOM	9437	N	GLN	455	114. 608 46. 332 56. 051 1. 00 19. 11 B	N
ATOM	9438	CA	GLN	455	114. 692 45. 305 55. 015 1. 00 14. 77 B	C
ATOM	9439	CB	GLN	455	113. 881 44. 085 55. 457 1. 00 13. 34 B	C
ATOM	9440	CG	GLN	455	114. 425 43. 413 56. 711 1. 00 12. 92 B	C
ATOM	9441	CD	GLN	455 455	113. 425 42. 482 57. 387 1. 00 13. 33 B	. C
ATOM	9442 9443		GLN GLN	455 455	112.514 41.958 56.749 1.00 14.25 B	0
ATOM ATOM	9444	C	GLN	455 455	113. 605 42. 266 58. 688 1. 00 13. 47 B 114. 156 45. 815 53. 669 1. 00 14. 10 B	N
ATOM	9445	0	GLN	455		C
ATOM	9446	N	TYR	456	114.058 45.059 52.704 1.00 14.35 B 113.803 47.094 53.597 1.00 13.95 B	O N
ATOM	9447	CA	TYR	456	113. 268 47. 651 52. 355 1. 00 13. 75 B	C
ATOM	9448	CB	TYR	456	111. 742 47. 600 52. 387 1. 00 13. 55 B	C
ATOM	9449	CG	TYR	456	111.049 47.707 51.045 1.00 10.86 B	Č
ATOM	9450		TYR	456	110.504 46.578 50.436 1.00 10.75 B	č
ATOM	9451	CE1	TYR	456	109. 815 46. 674 49. 236 1. 00 9. 29 B	č
ATOM	9452		TYR	456	110.891 48.941 50.405 1.00 9.71 B	Č
ATOM	9453		TYR	456	110. 207 49. 046 49. 200 1. 00 4. 15 B	C
ATOM	9454	CZ	TYR	456	109. 669 47. 910 48. 629 1. 00 8. 20 B	С
ATOM	9455	OH	TYR	456	108.949 47.994 47.464 1.00 11.71 B	0
ATOM	9456	С	TYR	456	113.718 49.092 52.190 1.00 14.04 B	С

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					P.I.C	4	104			(Continued)
					FIG	. 4 -	194			
ATOM	9457	0	TYR	456	113. 127	49. 991	52.775	1.00 15.30	В	0
ATOM	9458	N	TYR	457		49.309	51.382	1.00 15.11	В	N
ATOM	9459	CA	TYR	457		50.646	51.152	1.00 14.85	В	C
ATOM	9460	CB	TYR	457		50.674	51.390	1.00 14.57	В	C
ATOM	9461	CG	TYR	457	117. 271	50. 394	52. 786	1.00 14.62	В	C
ATOM			TYR	457		49. 088	53. 275	1.00 14.47	В	C
ATOM	9463		TYR	457		48. 836	54. 540	1.00 14.12	В	C
ATOM	9464		TYR	457		51.434	53. 595	1.00 13.34	В	C
ATOM	9465		TYR	457		51. 193 49. 902	54. 850 55. 318	1.00 13.51 1.00 11.72	B B	C C
ATOM ATOM	9466 9467	CZ OH	TYR TYR	457 457		49. 701	56. 559	1.00 11.72	В	0
ATOM	9468	С	TYR	457		51. 192	49. 742	1.00 15.66	В	C
ATOM	9469	Õ	TYR	457		50. 455	48. 797	1.00 17.46	В	ŏ
ATOM	9470	N	SER	458		52. 505	49.624	1.00 14.42	В	Ň
ATOM	9471	CA	SER	458		53. 207	48. 352	1.00 14.00	B	Ĉ
ATOM	9472	CB	SER	458		53. 950	48. 163	1.00 12.81	B	č
ATOM	9473	0G	SER	458		55. 138	48. 932	1.00 15.84	B	0
ATOM	9474	C	SER	458		54.175	48.620	1.00 15.10	В	C
ATOM	9475	0	SER	458		54. 431	49.791	1.00 14.29	В	0
ATOM	9476	N	VAL	459	116.946	54.709	47.574	1.00 13.45	В	N
ATOM	9477	CA	VAL	459		55. 593	47. 779	1.00 13.00	В	C
ATOM	9478	CB	VAL	459		54. 853	47. 433	1.00 13.28	В	C
ATOM	9479		VAL	459		54. 578	45. 934	1.00 10.72	В	Ċ
ATOM	9480		VAL	459		55. 672	47. 878	1.00 13.89	В	C
ATOM	9481	Ç	VAL	459		56. 882	46.969	1.00 14.23	В	C
ATOM	9482	0	VAL	459		57. 007	46.021	1.00 14.51	В	0.
ATOM	9483	N	SER	460		57. 834	47.347	1.00 14.01	В	N
ATOM	9484	CA	SER	460		59. 106 60. 116	46.643	1.00 14.81	В	C
ATOM ATOM	9485 9486	CB OG	SER SER	460 460		61.333	47. 272 46. 553	1.00 15.45 1.00 18.07	В	C
ATOM	9487	C	SER	460		59. 629	46. 693	1.00 15.07	B B	0 C
ATOM	9488	Ö	SER	460		60.040	47. 752	1.00 14.75	В	Ö
ATOM	9489	N	PHE	461		59.611	45. 547	1.00 14.10	В	N
ATOM	9490	ĊA	PHE	461		60.068	45.469	1.00 14.06	B	Č
ATOM	9491	CB	PHE	461		59. 229	44. 454	1.00 10.57	B	č
ATOM	9492		PHE	461				1.00 8.39	B	č
ATOM	9493		PHE	461		56.832	44. 792	1.00 7.71	B	č
ATOM	9494		PHE	461		57.444	45.367		В	Č
ATOM	9495	CE1	PHE	461	122.848	55.509	45.172	1.00 6.28	В	C
ATOM	9496		PHE	461	125.105	56.118	45.752	1.00 6.24	В	C
ATOM	9497		PHE	461		55. 153	45.653	1.00 6.94	В	C
ATOM	9498	C	PHE	461		61. 533	45.066	1.00 16.79	В	C
ATOM	9499	0	PHE	461		62.076	44. 340	1.00 17.81	В	0
ATOM	9500	N	SER	462		62. 170	45. 528	1.00 18.84	В	N
ATOM	9501	CA	SER	462		63. 555	45. 155	1.00 20.51	В	C
ATOM	9502	CB	SER	462		64. 137	46.036	1.00 21.92	В	C
ATOM	9503	OG C	SER	462		63. 421	45. 878	1.00 24.40	В	0
ATOM	9504	C	SER	462		63. 559		1.00 20.69	В	C
ATOM	9505	0	SER	462	124. 607	62. 505	43. 075	1.00 21.27	В	0

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					(Continued)
				FIG. 4-195	(
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9506 9507 9508 9509 9511 9511 9511 9511 9511 9511 9511	CA LYS CB LYS CC LYS CC LYS NZ LYS C LYS O LYS N GLU CA GLU CB GLU CB GLU CC GL	463 463 463 463 463 463 464 464 464 464	FIG. 4 - 195 124.708 64.736 43.128 1.00 22.99 B 125.109 64.846 41.728 1.00 25.69 B 125.483 66.291 41.401 1:00 27.00 B 124.275 67.189 41.270 1.00 30.44 B 124.427 68.146 40.097 1.00 35.16 B 123.083 68.756 39.718 1.00 37.88 B 123.169 69.566 38.471 1.00 40.00 B 126.204 63.904 41.230 1.00 26.63 B 126.057 63.297 40.169 1.00 27.72 B 127.305 63.777 41.959 1.00 27.45 B 128.355 62.868 41.502 1.00 28.40 B 129.710 63.576 41.429 1.00 31.19 B 130.079 64.030 40.027 1.00 35.17 B 130.079 64.030 40.027 1.00 35.17 B 129.150 65.100 39.495 1.00 37.56 B 129.200 66.229 40.022 1.00 41.38 B 128.371 64.817 38.557 1.00 38.51 B 128.476 61.627 42.367 1.00 26.36 B 127.404 61.302 43.081 1.00 23.96 B 127.404 61.302 43.081 1.00 22.56 B 128.362 60.245 45.074 1.00 20.68 B 128.362 60.245 45.074 1.00 20.68 B 128.365 69.244 45.591 1.00 16.26 B 128.661 61.476 45.462 1.00 22.56 B 129.588 61.693 46.562 1.00 24.73 B 130.041 63.154 46.609 1.00 25.44 B 131.173 63.405 47.581 1.00 22.56 B 129.588 61.693 46.562 1.00 24.73 B 130.041 63.154 46.609 1.00 25.44 B 131.173 63.405 47.581 1.00 29.20 B 131.835 64.762 47.351 1.00 32.39 B 127.544 61.314 47.846 1.00 22.52 B 128.859 61.318 47.847 1.00 24.27 B 129.469 60.850 48.809 1.00 24.32 B 127.544 61.514 47.846 1.00 22.52 B 126.722 61.182 49.004 1.00 23.27 B 126.356 62.441 49.794 1.00 23.00 B 127.527 63.237 50.292 1.00 24.92 B 128.201 64.119 49.451 1.00 25.30 B 129.301 64.841 49.904 1.00 25.30 B	(Continued) N C C C C C C C C C C C C C C C C C C
ATOM	9544	CD2 TYR	467	127. 981 63. 095 51. 604 1. 00 26. 01 B	C C
ATOM Atom	9545 9546	CE2 TYR CZ TYR	467 467	129. 079 63. 811 52. 064 1. 00 26. 37 B	C
ATOM	9547	OH TYR	467	129. 736 64. 681 51. 206 1. 00 26. 55 B 130. 841 65. 369 51. 645 1. 00 26. 89 B	C 0
ATOM	9548	C TYR	467	125. 428 60. 500 48. 584 1. 00 22. 16 B	Č
ATOM ATOM	9549 9550	0 TYR N TYR	467 468	125. 034 60. 557 47. 420 1. 00 22. 32 B	0
ATOM	9551	CA TYR	468	124. 775 59. 840 49. 534 1. 00 21. 72 B 123. 492 59. 208 49. 251 1. 00 21. 47 B	N
ATOM	9552	CB TYR	468	123. 492 59. 208 49. 251 1. 00 21. 47 B 123. 650 57. 817 48. 614 1. 00 19. 80 B	C C
ATOM	9553	CG TYR	468	124. 468 56. 797 49. 380 1. 00 19. 37 B	C
ATOM	9554	CD1 TYR.	468	125.844 56.683 49.184 1.00 20.24 B	Č

					(Continued)
		•		FIG. 4-196	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9555 9556 9556 9557 9558 9556 9562 9563 9564 9565 9566 9571 9573 9574 9577 9577 9578 9577 9578 9581 9583 9584 9585 9588 9588 9588 9588 9588 9588	CE1 TYR CD2 TYR CE2 TYR CZ TYR C TYR OH TYR C TYR O TYR N GLN CA GLN CB GLN CB GLN CCB GLN CCB GLN CCB GLN CCB CD1 CCB LEU CCD LEU CCA ARG CCA	468 468 468 468 469 469 469 469 469 470 470 470 470 471 471 471 471 471 471 471 471	126. 588 55. 695 49. 833 1. 00 20. 33 B 123. 856 55. 902 50. 252 1. 00 19. 91 B 124. 588 54. 915 50. 909 1. 00 20. 72 B 125. 951 54. 816 50. 695 1. 00 20. 60 B 126. 674 53. 845 51. 349 1. 00 20. 60 B 122. 602 59. 103 50. 474 1. 00 21. 65 B 123. 068 58. 836 51. 588 1. 00 19. 96 B 120. 369 59. 235 51. 355 1. 00 19. 96 B 120. 369 59. 235 51. 355 1. 00 18. 78 B 119. 277 60. 302 51. 283 1. 00 16. 79 B 118. 247 60. 143 52. 393 1. 00 16. 33 B 117. 035 61. 034 52. 214 1. 00 16. 44 B 116. 659 61. 739 53. 265 1. 00 18. 52 B 119. 729 57. 855 51. 240 1. 00 18. 75 B 119. 871 54. 860 53. 153 1. 00 18. 03 B 119.	C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM	9589 9590 9591 9592	0 ARG N CYS CA CYS C CYS	471 472 472 472	114.604 53.323 52.425 1.00 25.84 B 114.687 53.796 54.621 1.00 23.64 B 114.219 52.487 55.042 1.00 23.00 B	O N C
ATOM ATOM	9593 9594	O CYS CB CYS	472 472	112.732 52.636 55.321 1.00 21.14 B 112.323 53.547 56.036 1.00 21.12 B 114.981 52.073 56.299 1.00 23.91 B	C 0 C
ATOM ATOM ATOM	9595 9596 9597	SG CYS N SER	472 473	114.149 50.907 57.416 1.00 27.85 B 111.919 51.755 54.756 1.00 19.44 B	S N
ATOM ATOM ATOM	9598 9599	CA SER CB SER OG SER	473 473 473	110. 482 51. 846 54. 967 1. 00 18. 92 B 109. 789 52. 191 53. 646 1. 00 18. 36 B 110. 141 51. 261 52. 642 1. 00 21. 93 B	C C
ATOM ATOM	9600 9601	C SER O SER	473 473	109. 832 50. 609 55. 581 1. 00 17. 21 B 108. 615 50. 465 55. 530 1. 00 19. 59 B	0 C 0
ATOM ATOM	9602 9603	N GLY CA GLY	474 474	110. 629 49. 716 56. 156 1. 00 16. 48 B 110. 055 48. 532 56. 771 1. 00 16. 90 B	N C

		FIG. 4-197	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9605 O GLY 9606 N PRO 9607 CD PRO 9608 CA PRO 9609 CB PRO 9610 CG PRO 9611 C PRO 9612 O PRO 9613 N GLY	474 111.040 47.425 57.091 1.00 16.4 474 112.149 47.403 56.563 1.00 18.0 475 110.643 46.446 57.913 1.00 16.2 475 111.562 45.333 88.219 1.00 17.2 475 109.353 46.249 58.584 1.00 14.2 475 109.445 44.807 59.068 1.00 13.0 475 109.012 47.214 59.716 1.00 14.7 475 109.012 47.392 60.041 1.00 16.6 476 110.023 47.818 60.331 1.00 14.5 476 109.524 50.140 60.868 1.00 12.6 476 109.524 50.140 60.868 1.00 12.5 477 109.454 51.137 61.431 1.00 11.7 477 109.922 52.519 61.331 1.00 11.7 477 109.235 33.412 62.563 1.00 10.8 477 107.928 53.053	5 B O 5 B N 7 B C 6 B C 7 B C 7 B C 8 B C

(Continued)

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ATOM	9653	CA	THR	481	120. 129	58. 431	56.924	1.00 15.65	В	C
ATOM	9654	CB	THR	481	120.774	57.163	57.480	1.00 14.54	В	C
ATOM	9655	0G1	THR	481	120.459	56.065	56.622	1.00 18.10	В	0
								1.00 15.10	B	č
ATOM	9656	CG2	THR	481	120. 256	56.864	58. 858			
ATOM	9657	С	THR	481	120.964	58. 919.	55. 752	1.00 16.24	В	C
ATOM	9658	0	THR	481	120.650	58.648	54.602	1.00 16.93	В	0
ATOM	9659	N	LEU	482	122.035	59.646	56.058	1.00 18.90	В	N
ATOM	9660	CA	LEU	482	122.937	60.166	55.038	1.00 19.21	В	C
	9661	CB	LEU	482	123. 203	61.653	55. 279	1.00 20.10	B	Č
ATOM						62. 439	54. 092	1.00 20.10	В	Č
ATOM	9662	CG	LEU	482	123.765					
ATOM	9663		LEU	482	122.736	62. 475	52.975	1.00 21.10	В	C
ATOM	9664	CD2	LEU	482	124. 115	63.856	54.525	1.00 22.66	В	C
ATOM	9665	C	LEU	482	124.243	59.373	55. 121	1.00 19.39	В	C
ATOM	9666	0	LEU	482	124.684	59.013	56. 210	1.00 20.79	В	0
ATOM	9667	Ň	HIS	483	124.849	59.096	53.970	1.00 18.33	В	N
			HIS	483	126.090	58. 332	53. 903	1.00 16.79	B	Ĉ
ATOM	9668	CA								Č
ATOM	9669	CB	HIS	483	125. 791	56. 894	53. 488	1.00 14.55	В	
ATOM	9670	CG	HIS	483	124.697	56. 245	54. 276	1.00 14.89	В	C
ATOM	9671	CD2	HIS	483	123.358	56. 434	54. 264	1.00 15.13	В	C
ATOM	9672	ND1	HIS	483	124.933	55. 258	55. 211	1.00 16.09	В	N
ATOM	9673		HIS	483	123. 788	54.867	55.736	1.00 13.84	В	C
ATOM	9674		HIS	483	122.816	55. 565	55. 178	1.00 14.31	B	Ň
					127.043	58. 939	52. 868	1.00 18.94	B	Ċ
ATOM	9675	C	HIS	483						
ATOM	9676	0	HIS	483	126.617	59.665	51.961	1.00 19.56	В	0
ATOM	9677	N	SER	484	128.333	58. 645	53.003	1.00 19.52	В	N
MOTA	9678	CA	SER	484	129. 318	59. 131	52040	1.00 21.33	В	C
ATOM	9679	CB	SER	484	130.520	59.779	52. 738	1.00 21.77	В	С
ATOM	9680	0G	SER	484	131.351	58. 803	53. 344	1.00 24.25	В	0
ATOM	9681	C	SER	484	129.774	57. 907	51. 259	1.00 21.22	B	Č
ATOM	9682	0	SER	484	129.942	56.827	51.830	1.00 19.26	В	0
ATOM	9683	N	SER	485	129.979	58.076	49.960	1.00 22.12	В	N
ATOM	968 4	CA	SER	485	130. 389	56. 967	49.110	1.00 25.62	В	C
ATOM	9685	CB	SER	485	130.095	57. 301	47. 645	1.00 26.28	В	С
ATOM	9686	0G	SER	485	128.715	57. 552	47.444	1.00 30.40	В	0
ATOM	9687	Č	SER	485	131.840	56. 495	49. 221	1.00 26.33	В	Č
ATOM	9688	ŏ	SER	485	132.097	55. 300	49. 138	1.00 27.23	B	ŏ
								1.00 28.07		
ATOM	9689	N	VAL	486	132. 781	57. 416	49. 407		В	N
ATOM	9690	CA	VAL	486	134. 194	57.056	49.468	1.00 29.41	В	C
ATOM	9691	CB	VAL	486	135. 084	58. 284	49. 798	1.00 30.37	В	C
ATOM	9692	CG1	VAL	486	134. 786	58.797	51.192	1.00 31.49	В	С
ATOM	9693		VAL	486	136.553	57.909	49.665	1.00 30.81	В	C
ATOM	9694	C	VAL	486	134. 507	55. 929	50. 442	1.00 30.57	B	Č
	9695	0	VAL	486	135. 269	55.016	50. 119	1.00 31.62	В	Ö
ATOM										
ATOM	9696	N	ASN	487	133. 922	55. 979	51.630	1.00 30.95	В	N
ATOM	9697	CA	ASN	487	134. 159	54.928	52.610	1.00 31.75	В	C
ATOM	9698	CB	ASN	487	134.888	55. 498	53.833	1.00 35.87	В	C
ATOM	9699	CG	ASN	487	136.336	55.868	53. 537	1.00 38.55	В	С
ATOM	9700		ASN	487	136.838	56.895	54.014	1.00 38.47	В	Õ
ATOM	9701		ASN	487	137.019	55. 026	52. 759	1.00 37.49	B	Ň
UIOM	2101	NUL	אוטוז	401	101.013	JU. ULU	- LOS		U	14

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(Continued) FIG. 4-199 ATOM 9702 C **ASN** 132.850 54.288 53.048 1.00 30.74 C 487 132.830 53.486 9703 ASN 53.982 1.00 31.45 ATOM 0 487 В 0 9704 131.762 54.633 52.364 1.00 28.68 ATOM N **ASP** 488 В N 130.449 ATOM CA 54.108 52.707 1.00 26.66 9705 ASP 488 C В 130.331 CB **ASP** 488 52.636 52.313 1.00 27.90 ATOM 9706 C 52.440 9707 488 130.253 50.816 ATOM CG ASP 1.00 29.72 C ATOM 9708 OD1 ASP 129.461 53.146 50.161 488 1.00 31.30 В 0 130.977 ATOM 9709 OD2 ASP 488 51.572 50.290 1.00 32.18 130. 219 129. 654 54.259 54. 204 ATOM 1.00 25.72 9710 C ASP 488 В C **ATOM** 9711 0 ASP 488 53.382 54.856 1.00 24.30 B 0 9712 ATOM N LYS 489 130.669 55.378 54.754 1.00 25.25 В N ATOM 9713 LYS 130.503 55.610 CA 489 56.176 1.00 24.10 LYS ATOM 131.607 56.529 9714 CB 489 56.705 C 1.00 24.94 В **ATOM** 9715 CG LYS 489 131.622 57.898 56.069 1.00 29.19 C В **ATOM** 9716 LYS 132.805 58.719 CD 489 56.560 1.00 33.11 C В 55. 995 LYS 132. 771 133. 883 ATOM 9717 60.133 Č CE 489 1.00 34.94 В ATOM LYS 9718 NZ 60.959 56.541 1.00 39.70 489 N В ATOM 9719 C LYS 489 129.140 56.216 1.00 22.29 56.449 C В **ATOM** LYS 128.556 9720 0 489 56.872 55.585 1.00 20.15 0 128. 639 127. 352 ATOM 9721 GLY 55.968 N 490 57.657 1.00 22.04 B N 9722 **ATOM** CA **GLY** 490 56.487 58.067 1.00 20.03 В C ATOM 9723 C GLY 490 127.545 57.854 58.676 1.00 20.18 C В **ATOM** 9724 **GLY** 128.091 57.989 0 490 59.769 1.00 20.54 В 0 127. 092 127. 234 9725 58. 876 **ATOM** LEU N 491 57.965 1.00 19.44 В N 9726 LEU **ATOM** CA 491 60.233 58.440 1.00 19.54 В C ATOM 9727 491 CB LEU 127.032 61.203 1.00 20.53 57.283 C В 61.167 128. 153 127. 831 ATOM 9728 LEU CG 491 56.242 1.00 18.39 В C **ATOM** 9729 CD1 LEU 491 62.089 55.090 1.00 19.23 В C ATOM 9730 CD2 LEU 491 129.441 61.577 56.898 1.00 18.31 B C ATOM 9731 C LEU 491 126.287 60.555 59.586 1.00 20.91 C В 126.735 ATOM 9732 LEU 1.00 22.15 0 491 60.780 60.713 В 0 124.984 **ATOM** 9733 ARG N 492 60.566 59.316 1.00 20.73 В N ATOM ARG 9734 CA 492 124.020 60.881 60.364 1.00 20.06 В $^{\rm C}_{\rm C}$ **ATOM** 9735 CB ARG 124.036 492 62.382 60.644 1.00 20.71 ATOM 9736 CG 123.393 ARG 63.244 492 59.568 1.00 20.08 C ATOM ATOM 9737 CD ARG 123.759 492 64.698 59.798 1.00 21.15 C 9738 NE ARG 492 125.193 64.888 59.625 1.00 21.60 В N 125. 765 **ATOM** 9739 CZARG 492 65.192 58.466 1.00 23.12 В C ATOM 9740 NH1 ARG 492 125.022 65.360 57.380 1.00 24.47 В N ATOM 9741 NH2 ARG 492 127.083 65.286 58.383 1.00 23.72 N 122. 585 122. 247 ATOM 9742 C ARG 492 60.443 60.085 1.00 21.47 B C ATOM 9743 0 ARG 492 59.998 58.983 1.00 21.32 В 0 ATOM 9744 N VAL 493 121.746 60.580 61.107 1.00 20.97 В N ATOM 9745 VAL 493 CA 120.344 60.211 61.018 1.00 21.38 В C 119.883 **ATOM** 9746 CB VAL 493 59.537 62.325 1.00 22.41 B C ATOM 9747 VAL CG1 493 118.402 59.215 62.247 1.00 23.17 В C ATOM 9748 CG2 VAL 493 120.698 58.266 62.574 1.00 20.83 Č В 493 ATOM 9749 C VAL 119.497 1.00 21.55 61.456 60.763 C В

62.371 SUBSTITUTE SHEET (RULE 26)

61.580

119.462

1.00 21.85

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9750

ATOM

0

VAL

493

			FIG. 4-200	(Continued)
			1.10. 4-200	
ATOM ATOM		LEU 494 LEU 494	118.811 61.485 59.626 1.00 21.18 B	
ATOM		LEU 494 LEU 494	117. 974 62. 626 59. 264 1. 00 19. 43 B	
ATOM		LEU 494	110 101 00 010 50 050	
ATOM	9755 CD1 I		119.101 62.610 56.953 1.00 21.60 B 118.832 62.502 55.456 1.00 20.38 B	
ATOM	9756 CD2 I		119.929 63.851 57.271 1.00 19.91 B	
ATOM	9757 C I	LEU 494	116.615 62.576 59.964 1.00 18.58 B	
ATOM		EU 494	116.111 63.595 60.443 1.00 18.81 B	
ATOM		GLU 495	116. 025 61. 390 60. 022 1. 00 16. 24 B	
ATOM		ELU 495	114. 729 61. 225 60. 659 1. 00 16. 44 B	
ATOM ATOM		LU 495	113.612 61.651 59.698 1.00 17.53 B	C
ATOM		GLU 495 GLU 495	112. 217 61. 506 60. 268 1. 00 19. 67 B	
ATOM	9764 OE1 G		111.984 62.399 61.476 1.00 22.97 B 112.023 63.642 61.315 1.00 22.51 B	C
ATOM	9765 OE2 G		111 707 01 050 10	0
ATOM		LU 495	111.767 61.858 62.585 1.00 22.70 B 114.553 59.770 61.059 1.00 14.79 B	0
ATOM		LU 495	114. 678 58. 875 60. 236 1. 00 15. 37 B	C .
ATOM		SP 496	114. 264 59. 534 62. 329 1. 00 14. 29 B	N N
ATOM		SP 496	114.100 58.175 62.811 1.00 13.80 B	Č
ATOM		SP 496	115.128 57.867 63.909 1.00 14.57 B	č
ATOM		SP 496	114. 938 58. 715 65. 154 1. 00 12. 87 B	Č
ATOM ATOM	9772 OD1 A: 9773 OD2 A:		113. 849 59. 297 65. 330 1. 00 12. 34 B	0
ATOM			115. 882 58. 789 65. 971 1. 00 13. 20 B	0
ATOM		SP 496 SP 496	112. 711 57. 895 63. 341 1. 00 13. 42 B 112. 453 56. 808 63. 845 1. 00 14. 36 B	C
ATOM		SN 497	111 000 50 051 00 051	0
ATOM		SN 497	110 400 50 000 00 515	N
ATOM		SN 497	110. 460 58. 697 63. 717 1. 00 15. 91 B 109. 736 57. 666 62. 855 1. 00 16. 28 B	C
ATOM	9779 CG AS	SN 497	109. 227 58. 255 61. 564 1. 00 20. 09 B	C C
ATOM	9780 OD1 AS	SN 497	108. 308 59. 077 61. 570 1. 00 18. 95 B	0
ATOM	9781 ND2 AS		109. 829 57. 853 60. 443 1. 00 19. 49 B	Ň
ATOM	9782 C AS		110. 373 58. 292 65. 193 1. 00 17. 71 B	Ċ
ATOM ATOM	9783 0 AS		109. 591 57. 420 65. 564 1. 00 19. 20 B	0
ATOM	9784 N SE 9785 CA SE		111. 179 58. 924 66. 035 1. 00 18. 90 B	N
ATOM	9786 CB SE		111. 147 58. 627 67. 458 1. 00 20. 75 B 112. 210 59. 454 68. 191 1. 00 20. 93 B	Ċ
ATOM	9787 OG SE		110 401 50 050 40 005	C
ATOM	9788 C SE		100 700 50 050 00 000	0
ATOM	9789 0 SE		109. 760 58. 956 68. 020 1. 00 20. 54 B 109. 183 58. 184 68. 777 1. 00 20. 68 B	C
ATOM	9790 N AL		109. 238 60. 113 67. 637 1. 00 20. 46 B	O N
ATOM	9791 CA AL	A 499	107. 935 60. 564 68. 087 1. 00 21. 87 B	C
ATOM	9792 CB AL		107. 577 61. 858 67. 391 1. 00 21. 73 B	Č
ATOM	9793 C AL		106. 859 59. 520 67. 822 1. 00 23. 85 B	č
ATOM	9794 O AL		106. 279 58. 961 68. 758 1. 00 25. 77 B	Ö
ATOM ATOM	9795 N LE 9796 CA LE		106. 588 59. 262 66. 546 1. 00 23. 83 B	N
ATOM	9797 CB LE		105. 568 58. 286 66. 176 1. 00 24. 31 B	C
ATOM	9798 CG LEI		105. 642 57. 958 64. 678 1. 00 22. 08 B 104. 618 56. 922 64. 201 1. 00 20. 35 B	C
ATOM	9799 CD1 LEI		100 000 ==	C
-		- 500	103. 200 57. 349 64. 570 1. 00 19. 30 B	С

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(Continued) FIG. 4-201 **ATOM** 9800 CD2 LEU 500 104.744 56.763 62.721 1.00 19.60 $_{\rm C}^{\rm C}$ ATOM 9801 C LEU 500 105.745 57.009 66.974 1.00 24.37 В **ATOM** 9802 LEU 104.777 0 500 56.407 67.437 1.00 24.06 B 0 **ATOM** 9803 106.997 N ASP 56.601 501 67, 131 1.00 26.06 N В 107. 301 **ATOM** 9804 ASP CA 501 55.392 67.868 1.00 26.81 В C **ATOM** 9805 CB **ASP** 501 108.793 55. 1-20 67.844 1.00 25.74 В C **ATOM** 9806 CG ASP 109.145 53.848 501 68.556 1.00 26.66 В C **ATOM** OD1 ASP 9807 108.621 52.789 501 68.164 1.00 29.87 В 0 ATOM OD2 ASP 9808 501 109.939 53.901 69.512 1.00 30.35 В 0 ATOM 9809 C **ASP** 501 106.827 55.484 69.309 1.00 27.60 В C 106. 296 107. 011 **ATOM** 9810 0 **ASP** 501 54.520 69.855 1.00 27.99 В 0 ATOM 9811 LYS N 502 56.645 69.924 1.00 28.69 В N ATOM LYS 9812 CA 502 106.591 56.819 71.301 1.00 31.12 В C **ATOM** 9813 CB LYS 502 107.034 58.184 71.834 1.00 33.97 C В **ATOM** 9814 CG LYS 502 106.507 58.484 73.239 1.00 35.56 C В **ATOM** 9815 CD LYS 502 106.991 59.822 73.766 1.00 36.56 C В ATOM 9816 CE LYS 502 106.308 60.162 75.083 1.00 37.47 В C **ATOM** 9817 NZ LYS 502 106.514 59.098 76.104 1.00 38.22 В N **ATOM** 9818 105.080 C LYS 502 56.679 71.426 1.00 31.95 В **ATOM** 9819 0 LYS 502 104.592 55.937 B 72.276 1.00 33.49 0 9820 9821 ATOM N MET 503 104.338 57.380 70.574 1.00 32.49 В N ATOM CA MET 503 102.881 57.307 70.624 1.00 33.25 В C **ATOM** 9822 CB MET 503 102.254 58.342 69.690 1.00 35.92 B $^{\rm C}_{\rm C}$ ATOM 9823 CG MET 503 102.518 59.768 70.131 1.00 42.44 В ATOM 9824 SD MET 503 101.702 60.993 69.105 1.00 52.16 В S C C ATOM 9825 CE MET 503 100.419 61.581 70.243 1.00 50.62 B B ATOM 102. 361 9826 C 503 MET 55.927 70.279 1.00 31.30 ATOM 9827 0 MET 503 101.476 55.413 70.954 1.00 31.92 B 0 ATOM 9828 N LEU 504 102.914 55.318 69.238 1.00 30.00 В N ATOM 9829 CA LEU 504 102.471 53.99368.836 1.00 29.48 В C **ATOM** 9830 CB LEU 504 103.276 53.517 67.624 1.00 28.63 В **ATOM** 9831 CG LEU 504 102.517 66.290 53.477 1.00 29.55 B $\begin{array}{c} C \\ C \\ C \end{array}$ **ATOM** 54. 750 53. 300 9832 CD1 LEU 504 101.696 66.106 1.00 28.10 В **ATOM** CD2 LEU 9833 103.508 504 65.143 1.00 27.73 В **ATOM** 9834 C LEU 504 102.581 52.998 69.986 1.00 29.56 В C ATOM 9835 0 LEU 504 101.880 51.991 70.016 1.00 27.71 В 0 ATOM 9836 N GLN 505 103.458 53.291 70.938 1.00 31.52 В N ATOM 9837 CA GLN 505 103.641 52.425 72.096 1.00 33,96 В C ATOM 9838 CB GLN 505 104.829 72.927 52.915 1.00 36.96 В C **ATOM** 9839 CG GLN 505 106.167 52.836 72.200 Č 1.00 42.44 **ATOM** 9840 CD GLN 505 106.652 51.408 71.996 B 1.00 43.93 C **ATOM** 9841 0E1 GLN 505 107.079 50.746 72.943 1.00 45.80 В 0 ATOM 9842 NE2 GLN 505 50.925 106.581 70.758 1.00 45.49 В N ATOM 9843 C GLN 505 102.375 52.393 72.960 1.00 33.38 В C **ATOM** 9844 GLN 0 505 102.104 51.400 73.634 1.00 32.77 В 0 **ATOM** 9845 N ASN 506 101.607 53.482 72.928 1.00 32.89 N В **ATOM** 9846 CA ASN 506 73.694 100.362 53.590 1.00 32.38 В C **ATOM** 9847 CB ASN 506 99.997 55.062 73.937 1.00 35.05 В **ATOM** 9848

55.848 74.629

SUBSTITUTE SHEET (RULE 26)

1.00 39.34

C

CG

ASN

506

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ATOM ATOM ATOM	9849 9850 9851	ND2 C	ASN ASN ASN	506 506 506	101.426 101.703 99.208	55. 608 56. 796 52. 933	75. 799 73. 903 72. 936	1.00 41.09 1.00 39.00 1.00 30.32	B B B	O N C
ATOM	9852	0	ASN	506	98. 058	52. 995	73.377	1.00 30.93	B	O
ATOM	9853	N	VAL	507	99. 516	52. 305	71.803	1.00 26.94	B	N
ATOM	9854	CA	VAL	507	98. 497	51.664	70. 974	1.00 25.15	В	C
ATOM	9855	CB	VAL	507	98. 456	52.293	69. 545	1.00 23.88	В	
ATOM	9856	CG1	VAL	507	97. 287	51.730	68.755	1.00 21.31	B	C
ATOM	9857	CG2	VAL	507	98. 344	53.811	69.633	1.00 22.11	B	C
ATOM	9858	C	VAL	507	98. 717	50.164	70.825	1.00 25.62	B	C
ATOM	9859	0	VAL	507	99. 838	49.676	70.945	1.00 26.78	B	0
ATOM	9860	N	GLN	508	97. 639	49. 432	70. 567	1.00 25.89	B	N
ATOM	9861	CA	GLN	508	97. 730	47. 992	70. 381	1.00 25.14	B	C
ATOM	9862	CB	GLN	508	96. 486	47. 281	70. 917	1.00 27.32	B	C
ATOM	9863	CG	GLN	508	96. 322	47. 397	72. 422	1.00 29.65	B	C
ATOM ATOM	9864 9865	CD OE1		508 508	95. 190 95. 208	46. 543 45. 312	72. 958 72. 836	1.00 30.81 1.00 31.32	B B	C
ATOM	9866	NE2	GLN	508	94. 199	47. 190	73. 561	1.00 29.92	В	N
ATOM	9867	C		508	97. 869	47. 740	68. 899	1.00 23.65	В	C
ATOM	9868	O	GLN	508	96. 944	47. 277	68. 241	1.00 22.60	B	0
ATOM	9869	N	MET	509	99. 046	48. 063	68. 385	1.00 23.78	B	N
ATOM	9870	CA	MET	509	99. 347	47. 895	66. 980	1.00 23.48	B	C
ATOM	9871	CB	MET	509	100. 667	48. 578	66. 655	1.00 23.41	B	C
ATOM ATOM	9872 9873	CG SD	MET MET	509 509	100. 586 99. 279	50.070 50.681	66. 782 65. 719	1.00 26.19 1.00 28.03	B B	C S C
ATOM ATOM	9874 9875 9876	CE C	MET MET MET	509 509 509	100. 207 99. 425 99. 902	50. 994 46. 440 45. 599	64. 209 66. 579 67. 343	1.00 25.78 1.00 23.44 1.00 24.15	В В В	C O
ATOM ATOM ATOM	9877 9878	O N CD	PRO PRO	510 510	98. 951 98. 308	46. 121 47. 027	65. 365 64. 395	1.00 22.69 1.00 22.87	B B	N C
ATOM	9879	CA	PRO	510	98. 974	44. 751	64. 854	1.00 21.97	B	· C
ATOM	9880	CB	PRO	510	97. 987	44. 807	63. 701	1.00 22.62	B	
ATOM	9881	CG	PRO	510	98. 248	46. 171	63. 141	1.00 22.72	B	C
ATOM	9882	C	PRO	510	100. 381	44. 434	64. 379	1.00 21.20	B	C
ATOM	9883	Ŏ	PRO	510	101. 249	45. 301	64. 353	1.00 19.97	B	0
ATOM	9884	N	SER	511	100. 605	43. 188	63. 997	1.00 22.07	B	N
ATOM	9885	CA	SER	511	101.916	42. 782	63. 521	1.00 23.02	B	C
ATOM	9886	CB	SER	511	102.481	41. 654	64. 392	1.00 23.03	B	C
ATOM	9887	OG	SER	511	101.653	40.500	64. 358	1.00 26.12	B	0
ATOM	9888	C	SER	511	101.773	42.299	62. 094	1.00 23.35	B	C
ATOM	9889	O	SER	511	100. 659	42. 168	61.583	1.00 24.92	B	O
ATOM	9890	N	Lys	512	102. 906	42. 035	61.458	1.00 22.83	B	N
ATOM	9891	CA	LYS	512	102. 916	41.556	60.094	1.00 22.46	B	C
ATOM	9892	CB	LYS	512	103. 490		59.168	1.00 21.81	B	C
ATOM	9893	CG	LYS	512	103. 494	42. 209	57. 705	1.00 23.24	B	C
ATOM	9894	CD	LYS	512	103. 820		56. 851	1.00 24.28	B	C
ATOM	9895	CE	LYS	512	103. 824	43. 080	55. 393	1.00 23.13	В	C
ATOM	9896	NZ	LYS	512	104. 160	44. 299	54. 622	1.00 24.52	В	N
ATOM	9897	C	LYS	512	103. 742	40. 289	59. 993	1.00 22.87	В	C

					(Continued)
				FIG. 4-203	
ATOM	9898		512	104.803 40.180 60.585 1.00 23.26 B	0
ATOM	9899	N LYS	513	103. 235 39. 331 59. 235 1. 00 24. 10 B	N
ATOM	9900	CA LYS	513	103.910 38.069 59.039 1.00 24.49 B	C
ATOM	9901	CB LYS	513	103.046 36.923 59.566 1.00 25.52 B	С
ATOM	9902	CG LYS	513	103. 522 35. 537 59. 148 1. 00 26. 69 B	С
ATOM	9903	CD LYS	513	102. 493 34. 471 59. 522 1. 00 30. 85 B	Č
ATOM	9904	CE LYS	513	102. 805 33. 124 58. 866 1. 00 33. 37 B	C
ATOM	9905	NZ LYS	513	104. 131 32. 573 59. 287 1. 00 36. 04 B	N
ATOM	9906	C LYS	513	104. 143 37. 888 57. 552 1. 00 25. 44 B	C
ATOM	9907	0 LYS	513	103. 196 37. 871 56. 763 1. 00 27. 00 B	0
ATOM	9908	N LEU	514	105. 409 37. 771 57. 171 1. 00 24. 62 B	N
ATOM	9909	CA LEU	514	105.775 37.561 55.783 1.00 22.99 B	C
ATOM ATOM	9910	CB LEU CG LEU	514	106. 870 38. 536 55. 380 1. 00 22. 15 B	C
ATOM	9911 9912	CG LEU CD1 LEU	514 514	107. 307 38. 465 53. 925 1. 00 21. 19 B 106. 125 38. 790 53. 029 1. 00 19. 85 B	C
ATOM	9913	CD1 LEU	514		C C
ATOM	9914	C LEU	514	108. 438 39. 435 53. 701 1. 00 18. 42 B 106. 292 36. 132 55. 708 1. 00 24. 30 B	C
ATOM	9915	0 LEU	514	107.123 35.725 56.519 1.00 24.87 B	0
ATOM	9916	N ASP	515	105. 804 35. 361 54. 747 1. 00 25. 31 B	N N
ATOM	9917	CA ASP	515	106. 233 33. 975 54. 634 1. 00 26. 30 B	Č
ATOM	9918	CB ASP	515	105.599 33.156 55.757 1.00 28.58 B	č
ATOM	9919	CG ASP	515	106. 403 31. 929 56. 108 1. 00 30. 08 B	č
ATOM	9920	OD1 ASP	515	107. 209 31. 474 55. 272 1. 00 31. 89 B	Ŏ
ATOM	9921	OD2 ASP	515	106. 216 31. 409 57. 224 1. 00 33. 36 B	Ō
ATOM	9922	C ASP	515	105.805 33.414 53.282 1.00 26.17 B	Č
ATOM	9923	0 ASP	515	105. 343 34. 157 52. 417 1. 00, 26. 57 B	0
ATOM	9924	N PHE	516	105. 940 32. 104 53. 103 1. 00 25. 46 B	N
ATOM	9925	CA PHE	516	105. 571 31. 496 51. 838 1. 00 25. 82 B	С
ATOM	9926	CB PHE	516	106.792 31.384 50.930 1.00 23.83 B	C
ATOM	9927	CG PHE	516	107. 811 30. 395 51. 413 1. 00 22. 29 B	Č
ATOM	9928	CD1 PHE	516	108. 896 30. 808 52. 176 1. 00 22. 68 B	C
ATOM ATOM	9929 9930	CD2 PHE CE1 PHE	516	107. 678 29. 042 51. 119 1. 00 21. 58 B	C C C C C
ATOM	9931	CE2 PHE	516 516	109. 836 29. 885 52. 642 1. 00 21. 89 B	C
ATOM	9932	CZ PHE	516	108.609 28.113 51.579 1.00 21.19 B 109.689 28.536 52.342 1.00 20.70 B	C
ATOM	9933	C PHE	516	109.689 28.536 52.342 1.00 20.70 B 104.955 30.117 51.954 1.00 26.95 B	C
ATOM	9934	0 PHE		105.063 29.452 52.980 1.00 28.94 B	0
ATOM	9935	N ILE	517	104. 307 29. 707 50. 872 1. 00 27. 35 B	N N
ATOM	9936	CA ILE	517	103. 697 28. 398 50. 755 1. 00 28. 12 B	C
ATOM	9937	CB ILE	517	102, 155 28, 470 50, 729 1 00 26 53 B	Č
ATOM	9938	CG2 ILE	517	' 101. 645 29. 073 52. 016 1. 00 27. 39 B	Ċ
ATOM	9939	CG1 ILE	517	101.682 29.296 49.537 1.00 27.43 B	č
ATOM	9940	CD1 ILE	517	100.175 29.486 49.486 1.00 26.37 B	č ·
ATOM	9941	C ILE	517	104. 202 27. 896 49. 411 1. 00 30. 13 B	C C C
ATOM	9942	0 ILE	517	104.575 28.697 48.551 1.00 29.21 B	Ö
ATOM	9943	N ILE	518	104. 239 26. 581 49. 228 1. 00 33. 16 B	N
ATOM	9944	CA ILE	518	104.709 26.029 47.969 1.00 36.01 B	С
ATOM	9945	CB ILE	518	105. 680 24. 867 48. 190 1. 00 36. 84 B	С
ATOM	9946	CG2 ILE	518	106. 133 24. 311 46. 845 1. 00 36. 94 B	С
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				FIC	3. 4 -	204			Continued
9947			518	106.884	25.349	49.000	1.00 38.21	В	C
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				101.753			1.00 39.71	В	Ċ
9954	CG	LEU	519	100.989	27.144	45.612	1.00 39.82	В	С
9955			519	100.051	28. 205	45.045	1.00 39.14	В	С
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	0	ASN	520	106.004	23.637	41.348	1.00 44.64	B	0
9967	N	GLU	521	106.097	22. 791	43. 431	1.00 44.10	В	N
9968	CA	GLU		107. 536			1.00 45.15	В	С
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9978	CB	THR	522	106.605	27.566	42.198	1.00 34.21	В	Č
9979	0G1	THR	522	107. 109	27.115	40.936	1.00 34.20	В	0
9980				106.866	29. 057	42.318	1.00 33.69	В	С
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9990	С	LYS				45.984	1.00 28.56		Ċ
9991	0	LYS	523	107. 256	31. 335	45. 173	1.00 29.36	В	0
9992	N	PHE	524	105.692	30. 711	46.661	1.00 25.40	В	N .
	CA								Ç .
									C
9995	UG	PHE	524	103. 565	31. 136	44.516	1.00 21.75	R	С
	9948 9949 9950 9951 9952 9953 9955 9956 9957 9962 9963 9964 9965 9966 9967 9968 9969 9970 9971 9972 9973 9974 9975 9977 9978 9977 9978 9979 9980 9981 9988 9989 9989 9990	9948 CD1 9949 C 9950 O 9951 N 9952 CA 9953 CB 9954 CG 9956 CD2 9957 C 9958 O 9959 N 9960 CA 9961 CB 9962 CG 9963 OD1 9965 C 9966 O 9967 N 9968 CA 9969 CB 9970 CG 9971 CD 9972 OE1 9973 OE2 9974 C 9975 CA 9978 CB 9979 OG1 9977 CA 9978 CB 9979 OG1 9979 OG1 9970 CG 9971 CD 9971 CD 9972 OE2 9971 CD 9972 OE1 9973 OE2 9974 C 9975 CA 9978 CB 9979 OG1 9979 CA 9979 CC 9971 CD 9970 CA 9971 CD 9971 CD 9971 CD 9971 CD 9972 OE1 9973 OE2	9948 CD1 ILE 9949 C ILE 9950 O ILE 9951 N LEU 9952 CA LEU 9953 CB LEU 9954 CG LEU 9955 CD1 LEU 9956 CD2 LEU 9957 C LEU 9958 O LEU 9959 N ASN 9960 CA ASN 9961 CB ASN 9962 CG ASN 9963 OD1 ASN 9964 ND2 ASN 9965 C ASN 9965 C ASN 9966 O ASN 9967 N GLU 9976 CG GLU 9977 CG GLU 9970 CG GLU 9971 CD GLU 9970 CG GLU 9971 CD GLU 9971 CD GLU 9972 OE1 GLU 9971 CD GLU 9977 CA THR 9978 CB THR 9979 OG1 THR 9979 OG1 THR 9979 OG1 THR 9979 CG LYS 9988 CE LYS 9988 CE LYS 9988 CE LYS 9989 NZ LYS 9988 CE LYS 9989 NZ LYS 9980 C LYS 9981 C THR 9979 OG1 THR 9979 OG1 THR 9979 OG1 THR 9970 CG GLU 9971 CA THR	9948 CD1 ILE 518 9949 C ILE 518 9950 O ILE 518 9951 N LEU 519 9952 CA LEU 519 9953 CB LEU 519 9954 CG LEU 519 9955 CD1 LEU 519 9956 CD2 LEU 519 9957 C LEU 519 9959 N ASN 520 9960 CA ASN 520 9961 CB ASN 520 9961 CB ASN 520 9961 CB ASN 520 9964 ND2 ASN 520 9965 C ASN 520 9966 O ASN 520 9967 N GLU 521 9968 CA GLU 521 9969 CB GLU 521 9970 CG GLU 521 9970 CG GLU 521 9971 CD GLU 521 9971 CD GLU 521 9971 CD GLU 521 9972 OE1 GLU 521 9973 OE2 GLU 521 9974 C GLU 521 9975 O GLU 521 9976 N THR 522 9977 CA THR 522 9978 CB THR 522 9979 OG1 THR 522 9979 OG1 THR 522 9979 OG1 THR 522 9981 C THR 522 9981 C THR 522 9981 C THR 522 9981 C THR 522 9982 O THR 522 9983 N LYS 523 9984 CA LYS 523 9985 CB LYS 523 9986 CG LYS 523 9987 CD LYS 523 9987 CD LYS 523 9989 NZ LYS 523 9989 NZ LYS 523 9989 NZ LYS 523 9989 NZ LYS 523 99990 C LYS 523 99991 O LYS 523 99991 O LYS 523 99991 O LYS 523	9947 CG1 ILE 518 106.884 9948 CD1 ILE 518 107.976 9949 C ILE 518 103.558 9950 O ILE 518 102.581 9951 N LEU 519 103.679 9952 CA LEU 519 102.663 9953 CB LEU 519 101.753 9954 CG LEU 519 100.989 9955 CD1 LEU 519 100.051 9956 CD2 LEU 519 100.051 9957 C LEU 519 103.388 9958 O LEU 519 104.028 9959 N ASN 520 103.299 9960 CA ASN 520 103.963 9961 CB ASN 520 103.385 9962 CG ASN 520 102.045 9963 OD1 ASN 520 101.871 9965 C ASN 520 101.871 9966 O ASN 520 101.871 9967 N GLU 521 106.097 9968 CA GLU 521 106.097 9968 CA GLU 521 107.536 9969 CB GLU 521 107.536 9969 CB GLU 521 107.536 9970 CG GLU 521 109.775 9971 CD GLU 521 109.775 9971 CD GLU 521 109.775 9975 O GLU 521 109.986 9974 C GLU 521 109.975 9975 O GLU 521 109.034 9976 N THR 522 106.605 9979 OG1 THR 522 107.014 9977 CA THR 522 106.055 9979 OG1 THR 522 106.959 9980 CG2 THR 522 106.605 9981 C THR 522 106.959 9982 O THR 522 106.959 9983 N LYS 523 107.727 9984 CA LYS 523 107.559 9985 CB LYS 523 108.940 9986 CG LYS 523 108.944 9987 CD LYS 523 107.556 9992 N PHE 524 105.692 9993 CA PHE 524 104.912 9994 CB PHE 524 103.529	9947 CG1 ILE 518 106.884 25.349 9948 CD1 ILE 518 107.976 24.296 9949 C ILE 518 103.558 25.534 9950 O ILE 518 102.581 25.000 9951 N LEU 519 103.679 25.730 9952 CA LEU 519 102.663 25.294 9953 CB LEU 519 100.989 27.144 9955 CD1 LEU 519 100.989 27.144 9955 CD1 LEU 519 100.051 28.205 9956 CD2 LEU 519 100.051 28.205 9956 CD2 LEU 519 100.194 26.107 9957 C LEU 519 103.388 24.763 9958 O LEU 519 104.028 25.524 9959 N ASN 520 103.299 23.453 9960 CA ASN 520 103.963 22.824 9961 CB ASN 520 103.963 22.824 9961 CB ASN 520 103.963 22.824 9961 CB ASN 520 102.045 22.726 9963 OD1 ASN 520 101.168 22.634 9964 ND2 ASN 520 101.168 22.634 9965 C ASN 520 101.871 22.312 9965 C ASN 520 105.452 23.114 9966 O ASN 520 101.871 22.312 9965 C ASN 520 105.452 23.114 9966 O ASN 520 106.004 23.637 9967 N GLU 521 106.097 22.791 9968 CA GLU 521 107.536 23.012 9969 CB GLU 521 107.536 23.012 9969 CB GLU 521 109.775 22.642 9971 CD GLU 521 109.034 24.810 9978 CB THR 522 107.014 25.378 9977 CA THR 522 107.014 25.378 9977 CA THR 522 107.014 25.378 9977 CA THR 522 107.014 25.378 9978 CB THR 522 107.014 25.378 9979 OG1 THR 522 107.559 29.206 9978 CB LYS 523 107.559 29.206 9985 CB LYS 523 108.940 29.490 9986 CG LYS 523 108.940 29.490 9987 CD LYS 523 108.940 29.490 9988 CE LYS 523 107.559 29.206 9989 NZ LYS 523 107.559 29.206 9985 CB LYS 523 107.559 29.206 9985 CB LYS 523 107.559 29.206 9985 CB LYS 523 107.559 29.206	9947 CG1 ILE 518 106.884 25.349 49.000 9948 CD1 ILE 518 107.976 24.296 49.169 9949 C ILE 518 103.558 25.534 47.114 9950 O ILE 518 102.581 25.000 47.624 9951 N LEU 519 103.679 25.730 45.808 9952 CA LEU 519 102.663 25.294 44.863 9953 CB LEU 519 101.753 26.461 44.474 9954 CG LEU 519 100.989 27.144 45.612 9955 CD1 LEU 519 100.989 27.144 45.612 9956 CD2 LEU 519 100.051 28.205 45.045 9957 C LEU 519 100.194 26.107 46.381 9957 C LEU 519 103.388 24.763 43.637 9958 O LEU 519 104.028 25.524 42.910 9959 N ASN 520 103.399 23.453 43.419 9960 CA ASN 520 103.963 22.824 42.285 9961 CB ASN 520 103.385 23.337 40.964 9962 CG ASN 520 103.385 23.337 40.964 9962 CG ASN 520 101.871 22.312 39.386 9964 ND2 ASN 520 101.168 22.634 41.498 9964 ND2 ASN 520 101.871 22.312 39.386 9965 C ASN 520 101.871 22.312 39.386 9966 O ASN 520 105.452 23.114 42.316 9967 N GLU 521 106.097 22.791 43.431 9968 CA GLU 521 107.536 23.012 43.562 9969 CB GLU 521 107.536 23.012 43.562 9969 CB GLU 521 108.272 22.387 42.369 9971 CD GLU 521 109.775 22.642 42.339 9973 OE2 GLU 521 107.536 23.012 43.562 9974 C GLU 521 107.536 23.012 43.562 9975 O GLU 521 109.775 22.642 42.339 9973 OE2 GLU 521 107.536 23.012 43.562 9974 C GLU 521 109.775 22.644 43.361 9975 O GLU 521 109.775 22.644 43.363 9977 CD GLU 521 109.775 22.642 42.339 9978 OE GLU 521 109.775 22.642 42.339 9979 OGI THR 522 107.014 25.378 43.283 9977 CA THR 522 107.596 23.776 40.361 9974 C GLU 521 109.9775 22.644 63.661 9975 O GLU 521 109.934 24.810 44.072 9978 OE HR 522 106.605 27.566 42.198 9980 CG THR 522 106.605 27.566 42.198 9981 C THR 522 106.605 27.566 42.198 9982 CD THR 522 106.605 27.566 42.198 9983 N LYS 523 107.559 29.206 46.245 9985 CB LYS 523 108.940 29.490 46.838 9987 CD LYS 523 108.940 29.490 46.838 9988 CE LYS 523 108.940 29.490 46.838 9987 CD LYS 523 108.940 29.490 46.838 9988 CE LYS 523 106.819 30.519 45.944 9999 N PHE 524 106.692 30.711 46.661 9993 CA PHE 524 104.912 31.934 46.517 9994 CB PHE 524 105.692 31.1637 45.929	9947 CG1 ILE 518 106.884 25.349 49.000 1.00 38.21 9948 CD1 ILE 518 107.976 24.296 49.169 1.00 40.77 9949 C ILE 518 103.558 25.534 47.114 1.00 37.38 9950 O ILE 518 102.581 25.000 47.624 1.00 38.97 9951 N LEU 519 103.679 25.730 47.624 1.00 38.97 9952 CA LEU 519 102.663 25.294 44.863 1.00 40.68 9953 CB LEU 519 100.989 27.144 45.612 1.00 39.71 9954 CG LEU 519 100.989 27.144 45.612 1.00 39.71 9955 CD1 LEU 519 100.051 28.205 45.045 1.00 39.19 9956 CD2 LEU 519 100.051 28.205 45.045 1.00 39.19 9957 C LEU 519 100.194 26.107 46.381 1.00 40.51 9958 O LEU 519 103.388 24.763 43.637 1.00 42.22 9958 O LEU 519 103.388 24.763 43.637 1.00 42.22 9958 O LEU 519 103.93 22.424 42.285 1.00 44.57 9960 CA ANN 520 103.299 23.453 43.419 1.00 43.53 9960 CA ANN 520 103.995 23.453 43.419 1.00 44.57 9961 CB ASN 520 103.385 23.337 40.964 1.00 46.39 9962 CG ASN 520 102.045 22.726 40.639 1.00 48.97 9963 ODI ASN 520 101.871 22.312 39.386 1.00 46.39 9965 C ASN 520 101.871 22.312 39.386 1.00 50.46 9965 C ASN 520 101.871 22.312 39.386 1.00 44.67 9966 O ASN 520 101.871 22.312 39.386 1.00 44.67 9967 N GLU 521 106.097 22.791 43.431 1.00 44.10 9968 CA GLU 521 106.97 22.791 43.431 1.00 44.10 9968 CA GLU 521 106.97 22.791 43.431 1.00 44.13 9960 CB GLU 521 108.272 22.387 42.388 1.00 44.19 9970 CG GLU 521 107.536 23.012 43.562 1.00 45.15 9977 CD GLU 521 100.877 22.791 43.431 1.00 44.10 9978 N GLU 521 100.975 22.642 42.339 1.00 58.04 9977 CD GLU 521 100.975 22.642 42.339 1.00 58.04 9977 CD GLU 521 109.775 22.642 42.339 1.00 58.04 9977 CD GLU 521 109.775 22.642 42.339 1.00 34.09 9977 CD GLU 521 109.775 22.642 42.339 1.00 34.09 9977 CD GLU 521 109.775 22.642 42.339 1.00 34.09 9978 CB THR 522 107.014 25.378 43.383 1.00 38.59 9977 CA THR 522 106.866 29.057 44.14664 1.00 22.37 9988 CB THR 522 106.866 29.057 44.14664 1.00 23.85 9989 CB THR 522 106.866 29.057 44.14664 1.00 23.75 9988 CB LYS 523 108.940 29.490 46.838 1.00 33.19 9989 CD THR 522 106.868 29.057 44.14664 1.00 23.85 9999 O THR 523 107.559 29.206 46.245 1.00 29.30 9988 CB LYS 523 108.894 29.490 46.838 1.	9947 CG1 ILE 518 106.884 25.349 49.000 1.00 38.21 B 9948 CD1 ILE 518 107.976 24.296 49.169 1.00 40.77 B 9949 C ILE 518 103.558 25.534 47.114 1.00 37.38 B 9950 O ILE 518 102.581 25.000 47.624 1.00 38.97 B 9951 N LEU 519 103.679 25.730 47.624 1.00 38.97 B 9952 CA LEU 519 102.663 25.294 44.863 1.00 40.68 B 9953 CB LEU 519 101.753 26.461 44.474 1.00 39.71 B 9954 CG LEU 519 100.989 27.144 45.612 1.00 39.82 B 9955 CD1 LEU 519 100.989 27.144 45.612 1.00 39.82 B 9956 CD2 LEU 519 100.989 27.144 45.612 1.00 39.14 B 9957 C LEU 519 100.989 27.144 45.612 1.00 39.14 B 9958 O LEU 519 100.194 26.107 46.381 1.00 40.51 B 9959 N ASN 520 103.99 23.453 43.419 1.00 42.60 B 9959 N ASN 520 103.963 22.824 42.85 1.00 44.57 B 9961 CB ASN 520 103.963 22.824 42.85 1.00 44.57 B 9962 CG ASN 520 103.963 22.824 42.285 1.00 44.57 B 9963 OD1 ASN 520 101.68 22.334 41.498 1.00 50.54 B 9964 ND2 ASN 520 101.68 22.3314 42.316 1.00 44.13 B 9966 C ASN 520 101.680 22.314 42.316 1.00 44.13 B 9966 C ASN 520 105.452 23.114 42.316 1.00 44.13 B 9967 N GLU 521 106.004 23.637 41.348 1.00 44.64 B 9967 N GLU 521 106.007 22.791 43.431 1.00 44.10 B 9970 CG GLU 521 107.536 23.012 43.562 1.00 45.15 B 9970 CG GLU 521 107.536 23.012 43.562 1.00 45.15 B 9970 CG GLU 521 107.536 23.114 42.316 1.00 44.10 B 9971 CD GLU 521 106.007 22.791 43.431 1.00 44.0 B 9972 OEI GLU 521 106.007 22.791 43.431 1.00 44.10 B 9973 OE2 GLU 521 109.775 22.642 42.39 1.00 54.49 B 9971 CD GLU 521 109.775 22.642 42.39 1.00 54.49 B 9973 OE2 GLU 521 109.775 22.642 42.80 1.00 43.53 B 9978 CB THR 522 106.605 27.566 42.198 1.00 34.21 B 9979 OG1 THR 522 106.085 27.566 42.198 1.00 34.21 B 9979 OG1 THR 522 106.085 27.566 42.198 1.00 34.21 B 9979 OG1 THR 522 106.085 27.566 42.198 1.00 34.63 B 9988 CC LYS 523 108.94 30.329 45.848 1.00 33.13 B 9989 NZ LYS 523 107.559 29.206 46.245 1.00 32.75 B 9989 CD LYS 523 108.94 30.329 44.50 1.00 33.13 B 9989 NZ LYS 523 107.569 30.711 46.661 1.00 22.61 B 9999 O LYS 523 106.602 30.711 46.661 1.00 25.40 B 99990 O LYS 523 106.602 30.711 46.661 1.00 25.40 B

					FIC	G. 4-	206			(Cont	inued)
ATON ATON		0 N	MET ILE	528 529	100. 471 98. 432	39. 845 40. 554	58. 720 58. 100	1.00 21.07 1.00 19.01	B B	0 N	
ATON		CA	ILE	529	98. 428	41.614	59. 082	1.00 13.01	В	Č	
ATON		CB	ILE	529	97. 718	42. 860	58. 540	1.00 16.80	В	Č	
ATON			ILE	529	97. 656	43. 937	59.615	1.00 13.98	В	Č	
ATON			ILE	529	98. 469	43. 368	57. 296	1.00 15.06	, B	Č	
ATON			ILE	529	99. 934	43. 701	57. 537	1.00 11.03	В	č	
ATON		C	ILE	529	97. 656	40. 969	60. 225	1.00 20.15	В	č	
ATON		ŏ	ILE	529	96. 457	40. 720	60. 124	1.00 20.94	В	ŏ	
ATON		Ň	LEU	530	98. 359	40.653	61. 302	1.00 21.19	В	Ň	
ATON		CA	LEU	530	97. 717	39. 985	62. 420	1.00 21.61	B	Ĉ	
ATOM		CB	LEU	530	98. 649	38. 907	62. 976	1.00 19.85	B	č	
ATON		CG	LEU	530	99.086	37. 875	61.931	1.00 19.34	B	Č	
ATON			LEU	530	100. 238	37.027	62.461	1.00 20.33	В	C	
ATOM			LEU	530	97. 897	37.010	61.562	1.00 19.04	В	C	
ATON		С	LEU	530	97. 294	40.930	63. 521	1.00 22.34	В	С	
ATON		0	LEU	530	98.006	41.878	63.854	1.00 23.45	В	0	
ATON	1 10062	N	PR0	531	96. 104	40.697	64.088	1.00 23.19	В	N	
ATON		CD	PR0	531	95. 105	39.684	63. 711	1.00 22.71	В	С	
ATON		CA	PRO	531	95.600	41.545	65.169	1.00 24.33	В	С	
ATON		CB	PR0	531	94. 188	41.002	65. 404	1.00 22.74	В	С	
ATOM		CG	PR0	531	94. 276	39. 588	64.967	1.00 23.03	В	C	
ATON		C	PRO	531	96. 490	41.438	66. 407	1.00 25.18	В	Ç	
ATON		0	PRO	531	97. 244	40.478	66. 562	1.00 24.64	В	0	
ATON		N	PRO	532	96. 424	42. 433	67. 300	1.00 26.64	В	Ŋ	
ATON		CD	PRO	532	95. 502	43. 581	67. 326	1.00 25.36	В	C	
ATON		CA	PRO	532	97. 246	42. 397	68. 513	1.00 27.91	В	C	
ATON		CB	PRO	532	96. 868	43.698	69. 216	1.00 27.08	В	C	
ATON		CG	PRO	532	95. 443	43.897	68. 793	1.00 26.25	В	C	
ATON		C	PRO	532	96.945	41.160	69. 369	1.00 29.25	В	C	
ATON		0 N	PRO	532	95.865	40.579	69. 279	1.00 29.62	В	0	
ATON ATON		N CA	HIS HIS	533 533	97. 909 97. 738	40. 756 39. 602	70.187	1.00 30.65 1.00 31.99	В	N	
ATOM		CB	HIS	533	96. 749	39. 945	71.061 72.172	1.00 31.99	B B	C C	
ATOM		CG	HIS	533	96. 981	41. 293	72. 783	1.00 32.30	В	C	
ATON			HIS	533		42. 370		1.00 35.12	В	C	
ATON			HIS	533	98. 181	41.653	73. 358	1.00 35.18	В	N	
ATON			HIS	533	98. 096	42.892	73.807	1.00 36.37	В	C	
ATOM			HIS	533	96. 885	43. 350	73. 544	1.00 37.01	В	N	
ATON		C	HIS	533	97. 249	38. 382	70. 286	1.00 33.21	В	Č	
ATON		ŏ	HIS	533	96. 447	37. 590	70. 791	1.00 32.78	В	ŏ	
ATOM		Ň	PHE	534	97. 739	38. 243	69.058	1.00 33.50	В	Ň	
ATOM		CA	PHE	534	97. 374	37. 125	68. 200	1.00 34.63	B	Ċ	
ATOM		CB	PHE	534	98. 283	37.085	66.970	1.00 32.35	B	č	
ATOM		CG	PHE	534	97. 997	35.942	66.041	1.00 32.06	B	č	
ATOM	10090	CD1	PHE	534	96. 790	35.871	65.354	1.00 32.10	В	Č	
ATON	10091		PHE	534	98. 936	34. 938	65.848	1.00 32.66	В	Č	
ATOM		CE1		534	96. 522	34.819	64.486	1.00 31.59	В	С	
ATOM	1 10093	CE2	PHE	534	98. 679	33. 879	64.982	1.00 32.91	В	C	

									(Continued)
					FIG. 4-2	207			(Continued)
ATOM	10094	CZ	PHE	534	97.469 33.820	64. 298	1.00 32.93	В	С
ATOM	10095		PHE	534		68.941	1.00 36.77	В	Ċ
ATOM	10096	0	PHE	534		69. 565	1.00 37.84	В	0
ATOM	10097	N	ASP	535		68.868	1.00 39.07	В	N
ATOM	10098	CA	ASP	535		69. 523	1.00 40.37	В	С
ATOM	10099	CB	ASP	535		70.655	1.00 42.55	В	C
ATOM	10100	CG	ASP	535		71.465	1.00 45.66	В	Č
ATOM	10101		ASP	535		72. 445	1.00 49.45	В	0
ATOM	10102		ASP	535		71.125	1.00 46.59	В	0
ATOM	10103	C	ASP	535		68. 503	1.00 39.36	В	C
ATOM ATOM	10104 10105	O N	ASP LYS	535 536		67. 996	1.00 39.17	В	0
ATOM	10105	CA	LYS	536		68. 216 67. 233	1.00 40.23 1.00 41.20	В	N C
ATOM	10107	CB	LYS	536		66. 947	1.00 41.20	B B	C
ATOM	10108	CG	LYS	536		65. 731	1.00 42.02	В	C C
ATOM	10109	CD	LYS	536		65. 355	1.00 40.15	В	Č
ATOM	10110	CE	LYS	536		64. 040	1.00 48.68	В	Č
ATOM	10111	NZ	LYS	536		34. 079	1.00 48.77	В	Ň
ATOM	10112	C	LYS	536		37. 607	1.00 40.95	B	Ċ
ATOM	10113	0	LYS	536		66.778	1.00 41.99	B	Ŏ
ATOM	10114	N	SER	537		38. 848	1.00 40.73	B	Ň
ATOM	10115	CA	SER	537		39. 296	1.00 40.33	В	C
ATOM	10116	CB	SER	537	94. 598 28. 438 7	70.805	1.00 40.23	В	Ċ
ATOM	10117	0G	SER	537		71.541	1.00 40.12	В	0
ATOM	10118	C	SER	537		88.968	1.00 40.20	В	C
ATOM	10119	0	SER	537		88. 977	1.00 40.87	В	0
ATOM	10120	N	LYS	538		8. 674	1.00 39.23	В	N
ATOM	10121	CA	LYS	538	91.666 31.067 6	88. 337	1.00 37.32	В	C
ATOM	10122	CB	LYS	538	91.629 32.517 6	8. 817	1.00 39.07	В	Č
ATOM ATOM	10123 10124	CG CD	LYS	538		70. 170	1.00 41.74	В	C
ATOM	10124	CE	LYS LYS	538 520		1.316	1.00 44.86	В	C
ATOM	10125	NZ	LYS	538 538		1.540	1.00 46.82	В	C
ATOM	10127	C	LYS	538		'2. 636 6. 819	1.00 47.36	В	N
ATOM	10128	ŏ	LYS	538		6. 101	1.00 35.00 1.00 34.33	В	C
ATOM	10129	Ň	LYS	539		6. 335	1.00 34.33	B B	O N
ATOM	10130		LYS	539			1.00 32.92	В	C
ATOM	10131	CB	LYS	539		4. 510	1.00 32.32	В	C
ATOM	10132		LYS	539			1.00 36.07	В	C
ATOM	10133	CD	LYS	539			1.00 39.32	В	Č
ATOM	10134	·CE	LYS	539			1.00 39.62	В	Č
ATOM	10135	NZ	LYS	539			1.00 39.49	B	Ň
ATOM	10136	C	LYS	539		4. 471	1.00 31.07	B	Ċ
ATOM	10137	0	LYS	539	88. 424 33. 087 6		1.00 30.44	B	Ö
ATOM	10138	N	TYR	540	90. 274 33. 356 6		1.00 27.48	B	Ň
ATOM	10139	CA	TYR	540		3. 165	1.00 24.82	В	Ċ
ATOM	10140	CB	TYR	540			1.00 23.82	В	Ċ
ATOM	10141		TYR	540			1.00 23.61	В	С
ATOM	10142	CD1	IIK	540			1.00 21.98	В	С
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					FIG.	4 -	208			(Continued)
ATOM	10143	CE1		540		34. 708	66.130	1.00 21.65	В	C
ATOM	10144	CD2		540		36. 863	65. 257	1.00 22.89	В	C
ATOM	10145	CE2		540		36. 955	66. 449	1.00 22.77	В	C
ATOM	10146	CZ	TYR	540		35. 875	66. 881	1.00 22.87	В	C
ATOM	10147	0H	TYR	540		35. 965	68.062	1.00 23.97	В	0
ATOM	10148	C	TYR	540		34. 694	61.749	1.00 23.62	В	C
ATOM	10149	0	TYR	540		33. 842	60. 925	1.00 23.93	В	0
ATOM	10150	N	PRO	541		35.660	61.452	1.00 21.89	В	N
ATOM	10151	CD	PRO	541	05 045 4	36.667	62.320	1.00 21.22	В	C
ATOM	10152	CA	PRO	541		35. 719	60.095	1.00 20.52	В	C
ATOM	10153	CB	PRO	541		36. 717	60. 228	1.00 20.30	В	C
ATOM	10154	CG	PRO	541		37. 629	61.317	1.00 20.36	В	C
ATOM	10155	C	PRO	541		36. 266	59. 276	1.00 19.86	В	C
ATOM	10156	0	PRO	541		36. 799	59.841	1.00 19.90	В	0
ATOM	10157	N	LEU	542		36. 147	57.961	1.00 19.38	В	N
ATOM	10158	CA	LEU	542		36. 655	57. 169	1.00 18.21	В	C
ATOM	10159	CB	LEU	542		35. 483	56. 741	1.00 18.98	В	C
ATOM	10160	CG	LEU	542		35. 768	55. 816	1.00 19.24	В	C
ATOM	10161		LEU	542		34. 721	56.025	1.00 17.89	В	C C
ATOM	10162		LEU	542		35.775	54. 374 55. 954	1.00 19.31 1.00 17.31	В	C
ATOM	10163	C	LEU	542		37.458	55. 282	1.00 17.31	B B	
ATOM	10164	0 N	LEU	542		37.087	55. 694	1.00 16.06	В	O N
ATOM	10165	N	LEU	543		38. 564 39. 430	54. 559	1.00 14.81	В	C
ATOM	10166	CA CB	LEU LEU	543 543		10. 872	55. 015	1.00 13.73	В	C
ATOM ATOM	10167	CG	LEU	543		41. 892	53. 886	1.00 12.33	В	C
ATOM	10168 10169		LEU	543		11. 497	53. 113	1.00 13.11	В	C
ATOM	10109		LEU	543		13. 294	54. 454	1.00 3.31	В	Č
ATOM	10170	CDZ	LEU	543		39. 415	53. 620	1.00 11.07	В	Č
ATOM	10171	Õ	LEU	543		39. 893	53.966	1.00 14.04	В	Ö
ATOM	10173	N	LEU	544		38. 866	52. 428	1.00 15.02	B	N
ATOM	10174	CA	LEU	544		38. 807	51. 480	1.00 16.19	В	Č
ATOM	10175	CB	LEU	544		37. 609	50. 539	1.00 16.13	В	č
ATOM	10176	CG	LEU	544		37. 231	49.608	1.00 14.93	B	č
ATOM	10177		LEU	544		36. 752	50. 429	1.00 15.36	В	č
ATOM	10178		LEU	544		36. 128	48.654	1.00 15.79	B	č
ATOM	10179	C	LEU	544		40. 109	50.679	1.00 16.49	В	č
ATOM	10180	ŏ	LEU	544		10. 374	49.819	1.00 17.02	В	ŏ
ATOM	10181	Ň	ASP	545		10. 925	50. 997	1.00 15.13	B	Ň
ATOM	10182	CA	ASP	545		12.186	50. 306	1.00 14.91	B	Ċ
ATOM	10183	CB	ASP	545		13.069	51.117	1.00 15.71	B	č
ATOM	10184	CG	ASP	545		14. 434	50. 483	1.00 15.88	B	č
ATOM	10185		ASP	545		14. 641	49. 324	1.00 14.36	B	ŏ
ATOM	10186		ASP	545		15. 304	51.144	1.00 15.41	B	ŏ
ATOM	10187	Č	ASP	545		11.757	49.004	1.00 14.61	B	č
ATOM	10188	Ö	ASP	545		11.135	49.014	1.00 13.17	B	ŏ
ATOM	10189	N	VAL	546		12.098	47.881	1.00 15.03	\tilde{B}	Ň
ATOM	10190	CA	VAL	546		11.667	46.614	1.00 17.39	В	Ċ
ATOM	10191	CB	VAL	546			46.014	1.00 19.44	В	C
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										(Continued)
					FIC	G. 4-	209			(Collainaea)
ATOM	10192		I VAL	546	93.717	40. 124	44.647	1.00 17.87	В	Ç
ATOM	10193		2 VAL	546	93. 109		46. 983	1.00 20.93	В	C
ATOM	10194		VAL	546	94. 343		45. 542	1.00 17.09	В	C
ATOM	10195	0	VAL	546	93. 601	43.694	45. 447	1.00 18.12	В	0
ATOM	10196	N	TYR	547	95. 391	42.519	44. 745	1.00 15.70	В	N
MOŢA MOTA	10197 10198	CA CB	TYR TYR	547 547	95. 670 96. 838	43. 378 44. 335	43. 595	1.00 14.90	В	C
ATOM	10198	CG	TYR	547	97. 008	44. 333	43. 821 42. 622	1.00 12.56 1.00 12.84	B B	C C
ATOM	10200	CD1		547	98. 064	45. 063	41.727	1.00 12.04	В	C
ATOM	10201		TYR	547	98. 165	45.839	40. 578	1.00 12.01	В	Č
ATOM	10202		TYR	547	96. 057	46. 226	42. 331	1.00 11.82	В	Č
ATOM	10203		TYR	547	96. 149	47.002	41. 183	1.00 8.62	В	č
ATOM	10204	CZ	TYR	547	97. 204	46.804	40.314	1.00 10.60	B	Č
ATOM	10205	0H	TYR	547	97. 304	47.573	39.179	1.00 12.10	В	Ō
ATOM	10206	C	TYR	547		42.392	42.485	1.00 13.60	В	C
ATOM	10207	0	TYR	547	95. 244	42. 205	41.548	1.00 13.39	В	0
ATOM	10208	N	ALA	548	97. 170	41.763	42.608	1.00 13.66	В	N
ATOM	10209	CA	ALA	548	97. 594	40. 730	41.672	1.00 14.14	В	C
ATOM	10210	CB	ALA	548	96.658	39. 518	41.807	1.00 11.57	В	C
ATOM	10211	C	ALA	548	97. 732	41.105	40. 207	1.00 13.67	В	C
ATOM ATOM	10212 10213	O N	ALA	548	97. 681	40. 234	39. 340	1.00 14.21	В	0
ATOM	10213	CA	GLY GLY	549 549	97. 905 98. 078	42. 386	39. 913	1.00 13.87	В	N
ATOM	10214	CA	GLY	549	99. 405	42. 765 42. 209	38. 524 38. 046	1.00 12.26	В	C
ATOM	10216	Õ	GLY	549	100. 179	41.717	38. 855	1.00 12.16 1.00 12.33	B B	C 0
ATOM	10217	Ň	PRO	550	99. 700	42. 256	36. 739	1.00 12.03	В	N N
ATOM	10218	CD	PRO	550	98. 853	42.760	35. 644	1.00 12.99	В	Č
ATOM	10219	CA	PRO	550	100. 969	41.736	36. 217	1.00 13.32	В	č
ATOM	10220	CB	PRO	550	100.863	42.007	34. 721	1.00 14.56	B	č
ATOM	10221	CG	PRO	550	99. 391	42.015	34.473	1.00 14.10	B	Č
ATOM	10222	C	PRO	550	102.166	42.459	36.832	1.00 13.86	В	Ċ
ATOM	10223	0	PRO	550	102. 248	43. 683	36. 785	1.00 13.45	· В	0
ATOM	10224	N	CYS	551	103.088	41.694	37. 405	1.00 14.79	В	N
ATOM	10225	CA	CYS	551	104. 283	42. 244	38. 027	1.00 15.51	В	C
ATOM	10226	CB	CYS	551	105.035	43. 139	37. 036	1.00 17.05	В	С
ATOM	10227	SG	CYS	551	106. 732	43. 567	37. 543	1.00 17.09	В	S
ATOM ATOM	10228 10229	C	CYS	551 551	103. 967	43. 018	39. 312	1.00 16.05	В	C
ATOM	10229	O N	CYS SER	551 552	104.693	43. 938	39. 702	1.00 15.36	В	0
ATOM	10230	CA	SER	552 552	102. 883 102. 494	42. 631 43. 268	39.976	1.00 15.15	В	N
ATOM	10232	CB	SER	552	102. 494	43. 208	41. 229 41. 425	1.00 14.65 1.00 14.47	В	C .
ATOM	10233	OG	SER	552	100. 550	43. 149	41. 425	1.00 14.47	B B	C .
ATOM	10234	Č	SER	552	103. 201	42.608	42. 418	1.00 14.33	В	C
ATOM	10235	Ŏ	SER	552	103. 882	41.585	42. 273	1.00 15.21	В	0
ATOM	10236	N	GLN	553	103. 048	43. 201	43. 594	1.00 14.73	B	N N
ATOM	10237	CA	GLN	553	103.654	42.647	44. 794	1.00 14.31	B	Č
ATOM	10238	CB	GLN	553	105. 138	43.017	44. 892	1.00 13.21	\tilde{B}	č
ATOM	10239	CG	GLN	553	105.852	42.332	46.056	1.00 15.05	В	č
ATOM	10240	CD	GLN	553	107. 359	42.585	46.090	1.00 15.66	В	C

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ATOM	10241	0E1		553	107.812	43.686	46.400	1.00 16.56	В	0
ATOM	10242	NE2		553	108. 138	41.556	45. 773	1.00 15.50	В	N
ATOM	10243		GLN	553	102. 921	43. 166	46.012	1.00 14.58	В	C
ATOM	10244		GLN	553	103. 148	44. 295	46. 434	1.00 14.77	В	O N
ATOM	10245		LYS	554	102.031	42.344	46.568	1.00 14.78	B B	C
ATOM	10246		LYS	554	101. 284	42.734	47.754	1.00 16.57	В	C
ATOM	10247		LYS	554	99. 817	42.318	47. 633 46. 630	1.00 17.81 1.00 18.63	В	C
ATOM	10248		LYS	554 554	99. 031 99. 047	43. 142 44. 612	47.000	1.00 18.05	В	č
ATOM	10249		LYS LYS	554 554	98. 228	44. 902	48. 261	1.00 18.33	В	č
ATOM ATOM	10250 10251		LYS	554	96. 769	44. 771	48. 035	1.00 13.33	В	Ň
ATOM	10252		LYS	554	101.890	42. 148	49.024	1.00 16.05	B	Ċ
ATOM	10253		LYS	554	101.424	42. 429	50.124	1.00 17.37	B	0
ATOM	10254	Ň	ALA	555	102.939	41.350	48.866	1.00 15.91	В	N
ATOM	10255	CA	ALA	555	103.622	40.730	50.004	1.00 15.84	В	C
ATOM	10256	CB	ALA	555	103.656	39. 210	49.833	1.00 15.51	В	C
ATOM	10257	C	ALA	555	105.041	41.246	50.142	1.00 14.91	В	C
ATOM	10258	0	ALA	555	105.954	40.691	49.539	1.00 15.57	В	0
ATOM	10259	N	ASP	556	105. 233	42.304	50.924	1.00 16.20	В	N
ATOM	10260	CA	ASP	55 6	106. 571	42.854	51.134	1.00 16.65	В	C
ATOM	10261	CB	ASP	556	106.801	44. 085	50. 243	1.00 17.94	В	C
ATOM	10262	CG	ASP	556	105. 750	45. 159	50.430	1.00 19.95	В	C
ATOM	10263	OD1		556	105.355	45. 429	51.583	1.00 22.16	В	0
ATOM	10264	OD2		556	105. 327	45. 751	49.415	1.00 21.01	В	0
ATOM	10265	C	ASP	556	106.862	43. 202	52. 597	1.00 16.87	В	·C
ATOM	10266	0	ASP	556	106.046	42.962	53. 480	1.00 15.15	B B	O N
ATOM	10267	N	THR	557 557	108. 039 108. 443	43. 762 44. 132	52. 847 54. 200	1.00 17.93 1.00 18.07	В	C
ATOM	10268	CA CB	THR THR	· 557	108. 443	43. 826	54. 396	1.00 18.59	В	Č
ATOM ATOM	10269 10270		THR	557	110. 687	44. 589	53. 454	1.00 20.98	В	ŏ
ATOM	10270		THR	557	110. 188	42. 358	54. 157	1.00 19.55	В	č
ATOM	10271	C	THR	557	108. 203	45.616	54. 531	1.00 17.89	B	č
ATOM	10273	ŏ	THR	557	108. 776	46. 151	55. 479	1.00 16.94	B	Ŏ
ATOM	10274	Ň	VAL	558	107. 348	46. 272	53.754	1.00 16.56	В	N
ATOM	10275	CA	VAL	558	107.049	47.682	53.964	1.00 14.93	В	С
	10276		VAL		106. 483	48.302	52.676	1.00 14.99	В	C
ATOM	10277	CG1		558	106.033	49. 733	52.940	1.00 13.18	В	C
ATOM	10278	CG2	VAL	558	107.544	48. 247	51.568	1.00 13.02	В	С
ATOM	10279	С	VAL	558	106. 058	47. 921	55. 109	1.00 15.99	В	C
ATOM	10280	0	VAL	558	105.060	47. 211	55. 238	1.00 13.36	В	0
ATOM	10281	N	PHE	559	106. 348	48. 923	55. 941	1.00 15.43	В	N
ATOM	10282	CA	PHE	559	105. 484	49. 269	57.069	1.00 14.56	В	C
ATOM	10283	CB	PHE	559	106. 303	49. 933	58. 173	1.00 12.72	В	C
ATOM	10284		PHE	559	105. 469	50. 504	59. 282	1.00 11.04	В	C
ATOM	10285		PHE	559	105.064	49.712	60.347	1.00 10.65	В	C C C
ATOM	10286		PHE	559	105.056	51.833	59. 244	1.00 12.10 1.00 8.83	B B	C
ATOM	10287		PHE	559	104. 260	50. 232 52. 360	61.356 60.252	1.00 0.03	B B	C
ATOM	10288 10289		PHE	559 550	104. 251	52. 300	61.307	1.00 10.43	В	C C
ATOM	10409	UL	PHE	559	103. 855	01.004	01.001	1.00 0.00	ע	U

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ATOM	10290		PHE	559	104.		50. 230			14.21	В	C	
ATOM	10291	0	PHE	559	104.		51. 255	56.000		14.64	В	0	
ATOM	10292		ARG	560	103.		49.907			13.77	В	N	
ATOM	10293		ARG	560	102.		50.744			14.06	В	C	
ATOM	10294	CB	ARG	560	101.		50.117			12. 20	В	C	
ATOM	10295	CG	ARG	560	102.		49. 988	53. 954		11.36	В	Č	
ATOM	10296	CD	ARG	560	101.		49. 421	52. 755		10.73	В	C	
ATOM	10297	NE	ARG	560	102.		48. 486	51.999		13.38	В	N	
ATOM	10298	CZ	ARG	560	103.		48. 828	51.002		14.76	В	C	
ATOM	10299		ARG	560	103.		50.090	50.614		19.68	В	N	
ATOM	10300		ARG	560	103.		47.915	50. 421		16.46	В	N	
ATOM	10301	C	ARG	560	100.		50.980	57. 486		14.74	В	Ç	
ATOM	10302	0	ARG	560	100.		50.100	58. 291		16.54	В	0	
ATOM ATOM	10303 10304	N CA	LEU	561	100.		52. 183	57. 483		13.62	В	N	
ATOM	10304	CA CB	LEU LEU	561 561	99.		52.551	58. 392		13.55	В	C	
ATOM	10306	CG	LEU	561	99. (100. (53.875	59.100		11.68	В	C	
ATOM	10307		LEU	561	100.		53. 872 55. 299	60. 189		12.53	В	C	\
ATOM	10308		LEU	561	100.		52. 934	60. 698 61. 319		10.22	B B	C C	
ATOM	10309	C	LEU	561	98.		52. 725	57. 475		10. 22	В	Č	
ATOM	10310	ŏ	LEU	561	97. 9		53. 734	56. 785		10.30	В	0	
ATOM	10311	N	ASN	562	97.		51.748	57. 465		12.69	В	N	
ATOM	10312	ĊA	ASN	562	96. (51.841	56. 577		15.06	В	Č	
ATOM	10313	CB	ASN	562	96.4		51. 267	55. 220		14.07	В	Č	
ATOM	10314	CG	ASN	562	96. 9		49.823	55. 318		14.26	В	Č	
ATOM	10315		ASN	562	97. 8		49.309	54. 407		15.38	В	ő	
ATOM	10316		ASN	562	96. 5		49. 157	56. 423		11.43	B	Ň	
ATOM	10317	C	ASN	562	94.8		51.139	57.086		14.89	B	Ċ	
ATOM	10318	0	ASN	562	94. 7		50.793	58. 260		16.50	B	Ŏ	
ATOM	10319	N	TRP	563	93. 8		50.936	56.178		15. 26	B	Ň	
ATOM	10320	CA	TRP	563	92. 6	16	50. 281	56.502		15.35	В	Ċ	
ATOM	10321	CB	TRP	563	91.7	70	50.132	55. 244		13.87	В	Č	
ATOM	10322	CG	TRP	563	90. 3		49.719	55. 511	1.00	15.58	В	C C C C	
ATOM	10323	CD2	TRP	563	89. 6	23	48.721	54.804	1.00	12.95	В	C	
ATOM	10324	CE2	TRP	563	88. 3	30	48.684	55. 369		13.17	В	C	
ATOM	10325	CE3		563	89. 9		47.856	53. 745		10.64	В		
ATOM	10326			563						13.99		C	
ATOM	10327	NE1		563	88. 2		49.617	56. 373		14.03	В	N	
ATOM	10328	CZ2		563	87. 3		47.816	54. 911		13. 35	В	C	
ATOM	10329	CZ3		563	88. 9		46. 995	53. 290		9. 50	В	C	
ATOM ATOM	10330	CH2		563	87.6		46. 980	53. 872		12.48	В	C	
ATOM	10331 10332	C 0	TRP TRP	563	92. 8		48. 919	57. 119		16.18	В		
ATOM	10332		ALA	563	92. 2		48. 562	58. 132		15.81	В	0	
ATOM	10334		ALA	564 564	93.7		48. 161	56.515		17.44	В	N	
ATOM	10334		ALA	564	94.1		46.841	57.042		17.65	В	C	
ATOM	10336		ALA	564	95. 2		46. 186	56. 197		16.15	В	C	
ATOM	10337		ALA	564	94. 5 94. 2		46.973	58. 489		18.07	В	C	
ATOM	10338		THR	565	94. <i>2</i> 95. 3		46. 127 48. 037	59. 320 58. 793		18. 92 17. 73	B B	0 N	
- 14 714	10000	••						70. 193		11.10	D	N	•
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					FIG	. 4 -	2 1 2			(Commuca)
ATOM	10000	04	TITO	cer	05 017	40 9EN	CO 150	1 00 17 90	D	C
ATOM ATOM	10339 10340	CA CB	THR THR	565 565		48. 259 49. 551	60. 159 60. 294	1.00 17.29 1.00 17.13	B B	C C
ATOM	10340	0G1		565		49. 570	59. 330	1.00 20.36	В	Õ
ATOM	10341		THR	565		49.636	61.676	1.00 18.23	В	Č
ATOM	10342	C	THR	565		48. 355	61. 157	1.00 15.84	В	č
ATOM	10344	ŏ	THR	565		47. 804	62. 249	1.00 14.07	B	ŏ
ATOM	10345	Ň	TYR	566		49.061	60. 781	1.00 15.76	$\tilde{\mathtt{B}}$	Ň
ATOM	10346	CA	TYR	566		49. 204	61.664	1.00 17.74	B	Č
ATOM	10347	CB	TYR	566		50.335	61.177	1.00 15.61	В	Č
ATOM	10348	CG	TYR	566		50.039	61.311	1.00 17.40	В	С
ATOM	10349	CD1	TYR	566		49.688	60.195	1.00 17.77	В	C
ATOM	10350		TYR	566	87. 947	49.390	60.310	1.00 15.12	В	C
ATOM	10351		TYR	566		50.086	62.556	1.00 18.30	В	C
ATOM	10352		TYR	566		49. 789	62.682	1.00 17.35	В	C
ATOM	10353	CZ	TYR	566		49. 441	61.550	1.00 17.10	В	C
ATOM	10354	OH	TYR	566		49. 137	61.662	1.00 17.63	В	0
ATOM	10355	Ç	TYR	566		47. 899	61.777	1.00 19.12	В	C
ATOM	10356	0	TYR	566		47. 517	62. 871	1.00 20.12	В	0
ATOM	10357	N	LEU	567		47. 211	60.654	1.00 19.08	В	N
ATOM	10358		LEU	567		45. 959	60.648	1.00 19.66	В	C
ATOM	10359		LEU	567		45.419	59. 223	1.00 18.00	В	C
ATOM ATOM	10360 10361		LEU LEU	567 567		46. 252 45. 628	58. 284 56. 889	1.00 18.48 1.00 19.22	В	C
ATOM	10361		LEU	567		46. 325	58. 835	1.00 19.22	B B	C C
ATOM	10362	C	LEU	567		44. 898	61.544	1.00 10.78	В	C
ATOM	10364	ŏ	LEU	567		44. 102	62. 157	1.00 23.88	В	0
ATOM	10365	N	ALA	568		44. 883	61.628	1.00 19.62	В	N
ATOM	10366	CA	ALA	568		43. 898	62.466	1.00 20.08	В	Ċ
ATOM	10367	CB	ALA	568		43.601	61.907	1.00 18.06	B	č
ATOM	10368	Č	ALA	568		44. 362	63. 924	1.00 20.52	B	č
ATOM	10369	0	ALA	568		43.569	64.849	1.00 20.37	B	Õ
ATOM	10370	N	SER	569		45.653	64.128	1.00 20.79	B	N
ATOM	10371	CA	SER	569		46.182	65.474	1.00 21.75	В	Ċ
ATOM	10372	CB	SER	569	94. 520	47. 545	65.401	1.00 21.85	В	С
ATOM	10373	0G	SER	569		48. 188	66.657	1.00 22.64	В	0
ATOM	10374	C	SER	569		46. 297	66.267	1.00 22.83	В	C
ATOM	10375	0	SER	569		46. 029	67.470	1.00 22.38	В	0
ATOM	10376	N	THR	570		46.679	65.589	1.00 22.26	В	N
ATOM	10377	CA	THR	570		46.862	66. 232	1.00 21.45	В	С
ATOM	10378	CB	THR	570		48. 191	65.797	1.00 19.91	В	C
ATOM	10379	0G1		570		49. 285	66. 188	1.00 21.12	В	0
MOTA	10380	CG2		570 570		48. 351	66. 430	1.00 17.96	В	C
ATOM	10381	C	THR	570		45.751	65. 974	1.00 24.43	В	C
ATOM	10382 10383	0 N	THR	570 571		45.301	66. 894	1.00 27.79	В	0
ATOM ATOM	10384		GLU	571 571		45.317	64.727	1.00 23.34 1.00 21.95	B	N
ATOM	10385		GLU GLU	571 571		44. 280 44. 481	64. 415 62. 998	1.00 21.95	B B	C
ATOM	10386		GLU	571			62. 709	1.00 22.63	B B	C C
ATOM	10387		GLU	571			63. 696	1.00 24.03	В	C
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ATOM	10388	OE1 G	LU 571	85. 23	86 45.509	64. 258	1.00 28.12	В	0
ATOM	10389	OE2 G	LU 571	85.83	47.580	63.897	1.00 26.28	В	0
ATOM	10390	C G	LU 571	88.60			1.00 21.35	В	С
ATOM	10391		LU 571	87.90			1.00 19.91	В	0
ATOM	10392		SN 572	89.88			1.00 22.55	В	N
ATOM	10393		SN 572	90. 53			1.00 21.58	В	C
ATOM	10394		SN 572	89. 99			1.00 23.76	В	C
ATOM	10395		SN 572	90. 52			1.00 27.80	В	C
ATOM	10396	OD1 A		90.05			1.00 30.34	В	0
ATOM	10397	ND2 A		91.52			1.00 30.31	·B	N
ATOM	10398		SN 572	90.34			1.00 21.12	В	C
ATOM	10399		SN 572	90.11			1.00 20.16	В	0
ATOM	10400		LE 573	90.44			1.00 19.59	В	N C
ATOM ATOM	10401		LE 573 LE 573	90. 31 89. 50			1.00 18.06 1.00 18.14	B B	C C
ATOM	10402 10403	CG2 II		89. 37			1.00 18.14	В	C
ATOM	10403	CG1 II		88.14			1.00 18.33	В	C
ATOM	10405	CD1 II		87. 33			1.00 20.04	В	č
ATOM	10406		LE 573	91.70			1.00 18.47	В	č
ATOM	10407		LE 573	92. 48			1.00 19.08	В	ŏ
ATOM	10408		LE 574	92. 03			1.00 17.57	B	Ň
ATOM	10409		LE 574	93. 34			1.00 18.02	B	Č
ATOM	10410		LE 574	93.72			1.00 19.09	В	C
ATOM	10411	CG2 II	LE 574	94.95	0 37.280	58.870	1.00 20.13	В	C
ATOM	10412	CG1 II		94.00		61.172	1.00 21.02	В	С
ATOM	10413	CD1 II		94. 33			1.00 20.47	В	С
ATOM	10414		LE 574	93. 29			1.00 17.84	В	С
ATOM	10415		LE 574	92. 44		57.500	1.00 19.48	В	0
ATOM	10416		AL 575	94. 21			1.00 17.13	В	N
ATOM	10417		AL 575	94. 25			1.00 16.42	В	C
ATOM	10418		AL 575	94.35			1.00 16.55	В	C
ATOM ATOM	10419 10420	CG1 V		94. 27 93. 24			1.00 16.06	В	C
ATOM	10420	CG2 VA	AL 575 AL 575	95. 44 95. 45		57. 261	1.00 15.54	В	C
ATOM	10421		AL 575	96. 59		55. 786 56. 124	1.00 16.02 1.00 16.68	B B	C 0
ATOM	10423		LA 576	95. 18			1.00 16.08	В	N N
	10424			96. 24			1.00 15.22	В	
ATOM	10425		LA 576	96.06		54. 127	1.00 10.22	В	Č
ATOM	10426		LA 576	96. 33		52. 601	1.00 15.92	B	Č
ATOM	10427		LA 576	95. 39		52.046	1.00 16.20	B	ŏ
ATOM	10428		ER 577	97. 47		51.996	1.00 14.35	B	Ň
ATOM	10429		3R 577	97.72		50.606	1.00 13.57	B	Ċ
ATOM	10430		3R 577	98. 36		50.474	1.00 13.58	B	Č
ATOM	10431	OG SE	ER 577	97.45		50.866	1.00 16.22	В	Ŏ
ATOM	10432		ER 577	98.64		50.069	1.00 13.24	В	C
ATOM	10433	0 SE		99. 49		50. 788	1.00 13.05	В	0
ATOM	10434	N PI		98. 46		48.800	1.00 11.98	В	N
ATOM	10435	CA PI		99. 26		48. 183	1.00 11.24	В	Ċ
ATOM	10436	CB PF	E 578	98. 41	8 35.407	48.079	1.00 11.42	В	С

						(Continued)
					FIG. 4-214	
ATOM	10437	CG	PHE	578	99. 136 34. 232 47. 481 1. 00 10. 60 B	C
ATOM	10438		PHE	578	100. 196 33. 628 48. 152 1. 00 10. 29 B	C
ATOM	10439		PHE	578	98. 697 33. 679 46. 280 1. 00 10. 36 B	C
ATOM	10440		PHE	578	100. 805 32. 483 47. 640 1. 00 11. 15 B	C
ATOM	10441		PHE	578	99. 297 32. 537 45. 762 1. 00 11. 72 B	C
ATOM	10442	CZ	PHE	578	100.354 31.936 46.446 1.00 10.87 B	C
ATOM	10443	C	PHE	578	99. 746 37. 096 46. 805 1. 00 10. 56 B 99. 002 37. 704 46. 039 1. 00 10. 76 B	C 0
ATOM	10444	0 N	PHE	578 570	99.002 37.704 46.039 1.00 10.76 B 101.005 36.780 46.516 1.00 11.14 B	N N
ATOM ATOM	10445 10446	N CA	ASP ASP	579 579	101.617 37.069 45.227 1.00 9.94 B	Č
ATOM	10440	CB	ASP	579	103.008 37.682 45.401 1.00 9.15 B	č
ATOM	10448	CG	ASP	579	102.957 39.090 45.954 1.00 13.00 B	č
ATOM	10449		ASP	579	102.053 39.842 45.532 1.00 14.87 B	Ō
ATOM	10450		ASP	579	103. 816 39. 451 46. 796 1. 00 11. 19 B	0
ATOM	10451	C	ASP	579	101. 734 35. 741 44. 488 1. 00 11. 60 B	C
ATOM	10452	0	ASP	579	102. 633 34. 927 44. 753 1. 00 12. 07 B	0
ATOM	10453	N	GLY	580	100. 809 35. 510 43. 570 1. 00 10. 77 B	N
ATOM	10454	CA	GLY	580	100. 838 34. 274 42. 815 1. 00 11. 96 B	C
ATOM	10455	C	GLY	580	101. 458 34. 470 41. 450 1. 00 13. 34 B	C
ATOM	10456	0	GLY	580	102. 269 35. 376 41. 227 1. 00 12. 96 B	0
ATOM	10457	N	ARG	581	101. 080 33. 611 40. 521 1. 00 14. 18 B	N
ATOM	10458	CA	ARG	581	101. 615 33. 714 39. 187 1. 00 15. 34 B	C
ATOM	10459	CB	ARG	581	101.085 32.570 38.338 1.00 13.67 B	C
ATOM	10460	CG	ARG	581	101.809 31.283 38.666 1.00 15.30 B	C
ATOM	10461	CD	ARG	581	101.172 30.076 38.023 1.00 14.62 B 99.980 29.652 38.740 1.00 13.01 B	C N
ATOM ATOM	10462 10463	NE CZ	ARG ARG	581 581	99.186 28.672 38.330 1.00 13.69 B	C
ATOM	10403		ARG	581	99. 467 28. 024 37. 207 1. 00 13. 99 B	Ň
ATOM	10464		ARG	581	98. 112 28. 348 39. 036 1. 00 12. 41 B	N
ATOM	10466	C	ARG	581	101. 237 35. 069 38. 624 1. 00 17. 21 B	Č
ATOM	10467	Ŏ	ARG	581	100.175 35.615 38.934 1.00 17.96 B	ŏ
ATOM	10468	Ň	GLY	582	102.128 35.628 37.817 1.00 18.14 B	Ň
ATOM	10469	CA	GLY	582	101.868 36.933 37.258 1.00 17.73 B	С
ATOM	10470	C	GLY	582	102. 454 37. 998 38. 159 1. 00 16. 81 B	С
ATOM	10471	0	GLY	582	102.557 39.151 37.754 1.00 18.98 B	0
ATOM	10472	N	SER	583	102. 835 37. 625 39. 378 1. 00 15. 90 B	N
ATOM	10473	CA	SER	583	103. 423 38. 588 40. 309 1. 00 16. 60 B	C
ATOM	10474	CB	SER	583	103. 437 38. 024 41. 730 1. 00 17. 47 B	C
ATOM	10475	0G	SER	583	104. 229 36. 856 41. 811 1. 00 21. 54 B	0
ATOM	10476	C	SER	583	104. 841 38. 901 39. 841 1. 00 15. 56 B	C
ATOM	10477	0	SER	583	105. 389 38. 176 39. 013 1. 00 17. 79 B	0
ATOM	10478	N	GLY	584	105. 441 39. 970 40. 359 1. 00 14. 64 B	N
ATOM	10479	CA	GLY	584	106. 776 40. 334 39. 908 1. 00 13. 05 B 107. 969 40. 158 40. 831 1. 00 12. 28 B	C C
ATOM	10480	C	GLY	584 584	107. 969 40. 158 40. 831 1. 00 12. 28 B 107. 851 39. 648 41. 949 1. 00 11. 78 B	0
ATOM ATOM	10481 10482	O N	GLY TYR	、584 585	109.129 40.583 40.325 1.00 12.34 B	N N
ATOM	10483	CA	TYR	585	110.412 40.536 41.034 1.00 12.19 B	Č
ATOM	10484	CB	TYR	585	110.335 41.383 42.304 1.00 11.93 B	Č
ATOM	10485	CG	TYR	585	109.704 42.719 42.047 1.00 12.41 B	č
111 010		50		500	01/10/10/10/10/10/10/10/10/10/10/10/10/1	•

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					(Continued)
				FIG. 4-215	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10486 10487 10488 10489 10490 10491 10492 10493	CD1 TYR CE1 TYR CD2 TYR CE2 TYR CZ TYR OH TYR C TYR O TYR	585 585 585 585 585 585 585	110. 370 43. 694 41. 297 1. 00 12. 30 B 109. 756 44. 891 40. 979 1. 00 12. 43 B 108. 408 42. 983 42. 478 1. 00 10. 95 B 107. 783 44. 179 42. 167 1. 00 12. 28 B 108. 459 45. 126 41. 418 1. 00 13. 31 B 107. 831 46. 306 41. 109 1. 00 14. 33 B 110. 883 39. 141 41. 394 1. 00 12. 01 B 111. 673 38. 979 42. 319 1. 00 13. 01 B	C C C C O
ATOM ATOM ATOM ATOM ATOM	10494 10495 10496 10497 10498 10499	N GLN CA GLN CB GLN CG GLN CD GLN OE1 GLN	586 586 586 586 586	110.413 38.144 40.655 1.00 11.45 B 110.787 36.763 40.906 1.00 11.62 B 109.639 36.071 41.641 1.00 10.30 B 109.178 36.854 42.867 1.00 14.38 B 107.749 36.533 43.295 1.00 15.38 B 107.468 35.452 43.816 1.00 12.14 B	N C C C C
ATOM ATOM ATOM ATOM	10500 10501 10502 10503	NE2 GLN C GLN O GLN N GLY	586 586 586 587	106. 835 37. 478 43. 060 1. 00 15. 36 B 111. 118 36. 023 39. 602 1. 00 12. 85 B 111. 173 34. 786 39. 574 1. 00 13. 97 B 111. 336 36. 778 38. 525 1. 00 11. 70 B	N C O N
ATOM ATOM ATOM ATOM	10504 10505 10506 10507	CA GLY C GLY O GLY N ASP	587 587 587 588	111. 641 36. 168 37. 242 1.00 11.61 B 110. 405 35. 960 36. 373 1.00 14.10 B 109. 302 35. 786 36. 884 1.00 13. 91 B 110. 595 35. 949 35. 054 1.00 16. 19 B	C C O N
ATOM ATOM ATOM ATOM	10508 10509 10510 10511	CA ASP CB ASP CG ASP OD1 ASP	588 588 588 588	109. 500 35. 776 34. 105 1. 00 17. 70 B 110. 002 35. 993 32. 680 1. 00 18. 98 B 110. 708 37. 312 32. 505 1. 00 20. 57 B 110. 236 38. 335 33. 040 1. 00 23. 28 B	C C C
ATOM ATOM ATOM ATOM	10512 10513 10514 10515	OD2 ASP C ASP O ASP N LYS	588 588 588 589	111. 738 37. 327 31. 809 1. 00 23. 25 B 108. 723 34. 454 34. 139 1. 00 17. 46 B 107. 608 34. 389 33. 635 1. 00 16. 74 B 109. 294 33. 397 34. 697 1. 00 18. 02 B	0 C 0 N
ATOM ATOM ATOM ATOM	10516 10517 10518 10519	CA LYS CB LYS CG LYS CD LYS	589 589 589 589	108. 559 32. 143 34. 734 1. 00 20. 00 B 109. 383 31. 030 35. 372 1. 00 22. 21 B 108. 633 29. 710 35. 443 1. 00 27. 16 B 109. 526 28. 579 35. 940 1. 00 32. 47 B	C C C
ATOM ATOM ATOM ATOM	10520 10521 10522 10523	CE LYS NZ LYS C LYS O LYS	589 589 589 589	108. 753 27. 273 36. 111 1.00 33. 79 B 109. 605 26. 232 36. 771 1.00 35. 98 B 107. 290 32. 362 35. 536 1.00 20. 94 B 106. 244 31. 781 35. 242 1.00 23. 79 B	C N C O
ATOM ATOM ATOM ATOM	10524 10525 10526 10527	N ILE CA ILE CB ILE CG2 ILE	590 590 590 590	107. 384 33. 212 36. 552 1. 00 18. 06 B 106. 237 33. 523 37. 379 1. 00 14. 07 B 106. 681 33. 901 38. 814 1. 00 11. 33 B 105. 585 34. 654 39. 538 1. 00 9. 61 B	N C C C
ATOM ATOM ATOM ATOM	10528 10529 10530 10531	CG1 ILE CD1 ILE C ILE O ILE	590 590 590 590	107. 057 32. 635 39. 585 1. 00 10. 89 B 107. 750 32. 888 40. 897 1. 00 7. 05 B 105. 461 34. 682 36. 753 1. 00 15. 70 B 104. 254 34. 583 36. 511 1. 00 16. 31 B	C C C 0
ATOM ATOM ATOM	10532 10533 10534	N MET CA MET CB MET	591 591 591	106. 159 35. 774 36. 465 1. 00 15. 00 B 105. 506 36. 948 35. 907 1. 00 14. 79 B 106. 512 38. 088 35. 759 1. 00 14. 22 B	N C C

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(Continued)

					FIG	. 4 -	216			(Co
1 most	10505	00	ımm	504				1 00 10 55	ъ	0
ATOM	10535	CC	MET	591	105. 854 107. 027	39. 452 40. 830	35. 581 35. 526	1.00 18.55	B B	C
ATOM	10536 10537	SD CE	MET MET	591 591	107. 027	40. 502	33. 933	1.00 17.84 1.00 16.39	В	S
ATOM ATOM	10538	CE	MET	591	104. 788	36, 699	34. 582	1.00 10.39	В	C
ATOM	10536	0	MET	591	104. 766	37.113	34. 418	1.00 14.60	В	0
ATOM	10540	N	HIS	592	105. 451	36. 022	33. 647	1.00 14.45	В	N
ATOM	10540	CA	HIS	592	104. 863	35. 725	32. 343	1.00 14.00	В	Č
ATOM	10542	CB	HIS	592	105. 962	35. 424	31. 332	1.00 15.14	В	Č
ATOM	10543	CG	HIS	592	106. 753	36. 626	30. 922	1.00 17.56	B	Č
ATOM	10544		HIS	592	106.626	37. 933	31. 252	1.00 17.20	B	Č
ATOM	10545		HIS	592	107.810	36.555	30.041	1.00 17.84	В	N
ATOM	10546		HIS	592	108.300	37. 765	29.845	1.00 16.59	В	C
ATOM	10547	NE2	HIS	592	107. 598	38.620	30. 567	1.00 16.88	В	N
ATOM	10548	C	HIS	592	103. 859	34. 569	32.355	1.00 15.17	В	C
ATOM	10549	0	HIS	592	103. 224	34. 274	31. 344	1.00 15.89	В	0
ATOM	10550	N	ALA	593	103. 708	33. 917	33. 500	1.00 15.86	В	N
ATOM	10551	CA	ALA	593	102.775	32. 810	33. 615	1.00 14.02	В	C
ATOM	10552	CB	ALA	593	102.690	32. 353	35.060	1.00 13.60	В	C
ATOM	10553	C	ALA	593	101.393	33. 195	33. 106	1.00 15.66	В	C
ATOM ATOM	10554 10555	O N	ALA ILE	593 594	100. 647 101. 043	32. 335	32. 631 33. 207	1.00 17.83	В	0 N
ATOM	10556	CA	ILE	594 594	99. 731	34. 478 34. 945	32. 745	1.00 16.63 1.00 16.87	B B	N C
ATOM	10557	CB	ILE	594	99. 035	35. 857	33. 791	1.00 15.87	В	C
ATOM	10558		ILE	594	98. 506	35. 017	34. 932	1.00 16.36	В	Č
ATOM	10559		ÎLE	594	100.006	36. 915	34. 321	1.00 16.86	B	Č
ATOM	10560			594	100. 533	37. 882	33. 274	1.00 16.67	B	č
ATOM	10561	C	ILE	594	99. 748	35.689	31.413	1.00 17.96	$\tilde{\mathbf{B}}$	č
ATOM	10562	0	ILE	594	98. 884	36.525	31.160	1.00 19.03	В	0
ATOM	10563	N	ASN	595	100.718	35. 385	30.558	1.00 17.93	В	N
ATOM	10564	CA	ASN	595	100.802	36.050	29. 263	1.00 19.09	В	C
ATOM	10565	CB	ASN	595	102. 140	35. 737	28. 592	1.00 19.22	В	C
ATOM	10566	CG	ASN	595	102. 291	36. 441	27. 260	1.00 19.91	В	C
ATOM	10567		ASN	595	102. 320	37.668	27. 198	1.00 19.01	В	0
ATOM	10568		ASN	595	102. 377	35. 667	26. 184	1.00 19.95	В	N
ATOM ATOM	10569 10570	C	ASN	595 505	99.659	35.641	28. 330	1.00 19.09	В	C
ATOM	10570	O N	ASN ARG	595 506	99. 456 98. 933	34. 460 36. 630	28.076	1.00 19.31	В	0
ATOM	10572	CA	ARG	596 596	97. 799	36. 406	26. 911	1.00 19.66 1.00 20.07	В	N
ATOM	10573	CB	ARG	596	98. 212	35. 588	25. 677	1.00 20.07	B B	C
ATOM	10574	CG	ARG	596	99. 233	36. 247	24. 756	1.00 17.16	В	Č
ATOM	10575	CD	ARG	596	99. 655	35. 296	23. 636	1.00 17.14	В	Č
ATOM	10576	NE	ARG	596	98. 553	34. 982	22. 728	1.00 17.97	B	Ň
ATOM	10577	CZ	ARG	596	98. 102	35.816	21.795	1.00 19.85	B	Ċ
ATOM	10578	NH1	ARG	596	98.671	37.005	21.640	1.00 21.47	B	Ň
ATOM	10579		ARG	596	97.060	35.486	21.045	1.00 18.12	В	N
ATOM	10580	C	ARG	596	96. 692	35.655	27.632	1.00 21.03	В	С
ATOM	10581	0	ARG	596	95. 731	35. 213	27.005	1.00 22.67	В	0
ATOM	10582	N	ARG	597	96. 811	35. 529		1.00 20.90	В	N
ATOM	10583	CA	ARG	597	95. 831	34. 770	29. 714	1.00 20.85	В	C
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			(Continued)
		FIG. 4-217	
ATOM 10585 (ATOM 10586 (ATOM 10587 IATOM 10588 IATOM 10589 IATOM 10590 IATOM 10591 IATOM 10593 IATOM 10594 IATOM 10595 IATOM 10595 IATOM 10596 IATOM 10597 IATOM 10598 IATOM 10598 IATOM 10598 IATOM 10599 IATOM 10600 IATOM 10601 IATOM 10602 IATOM 10603 IATOM 10604 IATOM 10605 IATOM 10606 IATOM 10606 IATOM 10607 IATOM 10607 IATOM 10608 IATOM 10608 IATOM 10609 IATOM 10611 IATOM 10612 IATOM 10613 IATOM 10614 IATOM 10615 IATOM 10616 IATOM 10617 IATOM 10616 IATOM 10617 IATOM 10618 IATOM 10617 IATOM 10618 IATOM 10617 IATOM 10618 IATOM 10619 IATOM 10622 IATOM 10622 IATOM 10622 IATOM 10623 IATOM 10623 IATOM 10622 IATOM 10623 IATOM 1	N PHE 601 CA PHE 601 CB PHE 601 CC PHE 601 CD1 PHE 601 CE1 PHE 601 CE2 PHE 601 CCZ PHE 601	FIG. 4 - 217 96. 437 33. 414 30. 078 1. 00 23. 88 95. 850 32. 257 29. 300 1. 00 31. 40 95. 913 32. 520 27. 810 1. 00 34. 67 95. 006 31. 660 27. 059 1. 00 35. 49 94. 776 31. 792 25. 759 1. 00 35. 98 95. 386 32. 748 25. 075 1. 00 35. 20 93. 933 30. 974 25. 145 1. 00 39. 12 95. 292 35. 429 30. 976 1. 00 18. 83 94. 981 34. 739 31. 945 1. 00 17. 54 95. 175 36. 751 30. 964 1. 00 16. 66 94. 678 37. 477 32. 125 1. 00 15. 71 94. 482 38. 959 31. 769 1.00 12. 95 95. 523 39. 990 32. 248 1. 00 12. 69 96. 939 39. 473 32. 106 1. 00 1. 40 95. 361 41. 267 31. 466 1. 00 17. 19	B C C C C C C C C C C C C C C C C C C C
ATOM 10619 C ATOM 10620 C ATOM 10621 C	CE2 PHE 601 CZ PHE 601 C PHE 601	96. 949 28. 356 34. 581 1. 00 22. 61 97. 868 28. 427 33. 547 1. 00 20. 03 96. 346 32. 710 38. 244 1. 00 21. 61	B C B C B C
ATOM 10623 N ATOM 10624 C ATOM 10625 C			
ATOM 10627 C ATOM 10628 O ATOM 10629 O ATOM 10630 C	D GLU 602 E1 GLU 602 E2 GLU 602 GLU 602	94. 857 36. 847 36. 661 1. 00 17. 31 94. 930 35. 696 36. 184 1. 00 18. 92 94. 505 37. 830 35. 981 1. 00 16. 38 95. 111 34. 838 39. 952 1. 00 18. 97	B C B O B C
ATOM 10631 O ATOM 10632 N		95. 170 34. 953 41. 179 1. 00 18. 54 93. 979 34. 584 39. 296 1. 00 19. 02	B O B N

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				FIG. 4-218	(Continued)
ATOM	10633	CA VAL	603	92. 696 34. 413 39. 984 1. 00 21. 62 B	C
ATOM	10634	CB VAL	603	91. 513 34. 471 38. 999 1. 00 21. 51 B	C
ATOM	10635	CG1 VAL	603	90. 233 34. 055 39. 701 1. 00 19. 24 B	C
ATOM	10636	CG2 VAL	603	91. 380 35. 876 38. 442 1. 00 21. 00 B	C
ATOM	10637	C VAL	603	92. 643 33. 073 40. 716 1. 00 22. 35 B	. C
ATOM	10638	O VAL	603	92. 160 32. 989 41. 848 1. 00 21. 06 B	0
ATOM	10639	N GLU	604	93. 141 32. 031 40. 059 1. 00 22. 98 B	N
ATOM	10640	CA GLU	604	93. 182 30. 702 40. 656 1. 00 26. 04 B	C
ATOM	10641	CB GLU	604	93. 721 29. 681 39. 645 1. 00 28. 46 B	C
ATOM	10642	CG GLU	604	92. 956 29. 671 38. 326 1. 00 35. 94 B	C
ATOM	10643	CD GLU	604	93. 559 28. 742 37. 273 1. 00 40. 17 B	C
ATOM	10644	OE1 GLU	604	93. 215 28. 911 36. 076 1. 00 40. 47 B	0
ATOM	10645	OE2 GLU	604	94. 360 27. 844 37. 637 1. 00 41. 61 B	0
ATOM	10646	C GLU	604	94. 072 30. 705 41. 905 1. 00 24. 63 B 93. 657 30. 255 42. 976 1. 00 25. 47 B 95. 286 31. 234 41. 775 1. 00 22. 17 B	C
ATOM	10647	O GLU	604		O
ATOM	10648	N ASP	605		N
ATOM	10649	CA ASP	605	96. 213 31. 255 42. 900 1. 00 21. 12 B	C
ATOM	10650	CB ASP	605	97. 568 31. 827 42. 463 1. 00 23. 09 B	C
ATOM	10651	CG ASP	605	98. 263 30. 958 41. 414 1. 00 24. 43 B	C
ATOM ATOM ATOM	10652 10653 10654	OD1 ASP OD2 ASP C ASP	605 605 605	97. 894 29. 774 41. 266 1. 00 26. 59 B 99. 188 31. 453 40. 742 1. 00 25. 60 B 95. 712 31. 967 44. 159 1. 00 19. 42 B	0 C
ATOM	10655	0 ASP	605	96. 099 31. 598 45. 260 1. 00 19. 67	O
ATOM	10656	N GLN	606	94. 868 32. 983 44. 014 1. 00 17. 23 B	N
ATOM	10657	CA GLN	606	94. 337 33. 673 45. 192 1. 00 16. 41 B	C
ATOM	10658	CB GLN	606	93. 576 34. 951 44. 795 1. 00 17. 09 B	C
ATOM	10659	CG GLN	606	94. 407 36. 070 44. 165 1. 00 15. 81 B	C
ATOM	10660	CD GLN	606	95. 332 36. 748 45. 162 1. 00 15. 36 B	C
ATOM	10661	OE1 GLN	606	94. 879 37. 283 46. 173 1. 00 13. 19 B	O
ATOM	10662	NE2 GLN	606	96. 637 36. 730 44. 878 1. 00 14. 39 B	N
ATOM	10663	C GLN	606	93. 360 32. 706 45. 878 1. 00 15. 71 B	C
ATOM	10664	O GLN	606	93. 337 32. 583 47. 102 1. 00 14. 30 B	0
ATOM	10665	N ILE	607	92. 549 32. 030 45. 070 1. 00 13. 95 B	N
ATOM	10666	CA ILE	607	91. 584 31. 076 45. 583 1. 00 13. 95 B	C
ATOM	10667	CB ILE	607	90. 772 30. 437 44. 448 1. 00 12. 90 B	C
ATOM	10668	CG2 ILE	607	89. 925 29. 294 44. 996 1. 00 11. 78 B	C
ATOM	10669	CG1 ILE	607	89. 909 31. 504 43. 773 1. 00 12. 90 B	C
ATOM	10670	CD1 ILE	607	89. 162 31. 016 42. 560 1. 00 11. 00 B	C
ATOM	10671	C ILE	607	92. 330 29. 985 46. 318 1. 00 15. 04 B	C
ATOM	10672		607	92. 008 29. 670 47. 462 1. 00 15. 40 B	0
ATOM	10673	N GLU	608	93. 331 29. 413 45. 652 1. 00 16. 29 B	N
ATOM	10674	CA GLU	608	94. 144 28. 359 46. 246 1. 00 18. 48 B	C
ATOM	10675	CB GLU	608	95. 180 27. 864 45. 235 1. 00 18. 74 B	C
ATOM	10676	CG GLU	608	96. 164 26. 851 45. 792 1. 00 22. 43 B	C
ATOM	10677	CD GLU	608	95. 498 25. 557 46. 213 1. 00 29. 00 B	C
ATOM	10678	OE1 GLU	608	96. 096 24. 817 47. 032 1. 00 32. 52 B	0
ATOM	10679	OE2 GLU	608	94. 382 25. 274 45. 721 1. 00 31. 62 B	0
ATOM	10680	C GLU	608	94. 848 28. 889 47. 501 1. 00 20. 58 B	C
ATOM	10681	O GLU	608	95. 114 28. 138 48. 446 1. 00 23. 01 B	0

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					E I C		0.1.0			(Continued)
					FIG	. 4 -	219			
ATOM ATOM	10682 10683	N CA	ALA ALA	609 609	95. 150 95. 811	30. 183	47. 506 48. 646	1.00 19.99 1.00 21.28	В	N C
ATOM	10684	CB	ALA	609	96. 269	30. 789 32. 196	48. 310	1.00 21.28	B B	C
ATOM	10685	C	ALA	609	94. 826	30. 819	49. 797	1.00 21.63	В	č
ATOM	10686	0	ALA	609	95. 152	30.426	50.915	1.00 21.88	В	0
ATOM	10687	N	ALA	610	93. 618	31.286	49.516	1.00 23.07	В	N
ATOM	10688	CA	ALA	610	92. 580	31. 358	50. 535	1.00 25.56	В	C
ATOM ATOM	10689 10690	CB C	ALA ALA	610 610	91.317 92.300	31. 963 29. 952	49. 957 51. 024	1.00 25.38 1.00 26.13	B B	C C
ATOM	10691	Ö	ALA	610	92. 256	29. 694	52. 223	1.00 25.13	В	Ö
ATOM	10692	Ň	ARG	611	92.119	29. 044	50.073	1.00 28.12	В	Ň
ATOM	10693	CA	ARG	611	91.838	27.647	50.374	1.00 28.88	B	Č
ATOM	10694	CB	ARG	611	91.886	26.826	49.087	1.00 27.27	В	С
ATOM	10695	CG	ARG	611	91.518	25. 372	49. 260	1.00 28.40	В	C
ATOM ATOM	10696 10697	CD NE	ARG ARG	611 611	91.547 90.501	24.668	47. 925	1.00 30.54	В	C
ATOM	10698	CZ	ARG	611		25. 152 25. 223	47. 028 45. 706	1.00 33.73 1.00 36.39	B B	N C
ATOM	10699		ARG	611		24. 848	45. 129	1.00 38.00	В	Ň
ATOM	10700		ARG	611		25.645	44. 956	1.00 37.15	B	Ň
ATOM	10701	C	ARG	611		27.082	51.391	1.00 29.24	В	C
ATOM	10702	0	ARG	611		26. 330	52. 287	1.00 30.51	В	0
ATOM ATOM	10703 10704	N CA	GLN GLN	612 612		27. 452	51.260	1.00 30.24	В	N
ATOM	10704	CB	GLN	612		26. 965 27. 029	52. 182 51. 532	1.00 30.75 1.00 29.62	B B	C C
ATOM	10706	CG	GLN	612		25. 866	50. 581	1.00 23.02	В	C
ATOM	10707	CD	GLN	612		25. 741	50. 150	1.00 32.19	В	č
ATOM.	10708		GLN	612	99.097	25.778	50.979	1.00 32.20	В	Ō
ATOM	10709		GLN	612		25. 578	48. 848	1.00 31.86	В	N
ATOM	10710	C	GLN	612		27. 691	53. 524	1.00 31.36	В	C
ATOM ATOM	10711 10712	O N	GLN PHE	612 613		27. 095 28. 969	54. 545 53. 533	1.00 32.39	В	0
ATOM	10713	CA	PHE	613		29. 717	54. 784	1.00 31.39 1.00 30.50	B B	N C
ATOM	10714	CB	PHE	613		31. 217	54. 538	1.00 30.43	В	Č
ATOM	10715	CG	PHE	613		31.853	53.775	1.00 31.06	B	č
ATOM	10716		PHE	613		31.532	54.058	1.00 32.48	В	C
ATOM	10717		PHE	613	95. 385	32. 805	52. 796	1.00 30.25	В	C
ATOM ATOM	10718 10719	CE1 CE2		613 613		32.156	53.371	1.00 32.97	В	C
ATOM	10719		PHE	613		33. 432 33. 109	52. 109 52. 394	1.00 31.17 1.00 32.13	B B	C C
ATOM	10721	Č	PHE	613		29. 214	55. 607	1.00 30.36	В	C
ATOM	10722	0	PHE	613		29. 216	56. 830	1.00 28.96	B	ŏ
ATOM	10723	N	SER	614	92.478	28. 786	54. 923	1.00 31.88	В	N
ATOM	10724	CA	SER	614		28. 286	55.600	1.00 34.43	В	С
ATOM ATOM	10725 10726	CB OG	SER SER	614 614		28.104	54.607	1.00 34.30	В	C
ATOM	10720	C	SER	614 614		27. 055 26. 953	53. 697 56. 264	1.00 34.39 1.00 35.74	B	0 C
ATOM	10728	Õ	SER	614		26. 519	57. 178	1.00 35.74	B B	0
ATOM	10729	N	LYS	615		26. 307	55. 797	1.00 36.52	В	N N
ATOM	10730.	CA	LYS	615		25. 030	56.350	1.00 37.25	В	C

				DI	a 4	0.00			(Continued)
	. "•			F 1 (G. 4 -	220			
ATON ATON		CB LY CG LY			24. 196 23. 516	55. 283	1.00 37.94	В	C
ATON		CD LY			23. 050	54. 293 53. 053	1. 00 40. 25 1. 00 42. 18	B B	C C
ATON		CE LY			22. 317	53.419	1.00 42.76	В	Č
ATON		NZ LY			22. 147	52. 237	1.00 43.07	В	Ň
ATON		C LY			25. 231	57. 544	1.00 37.98	B	Ċ
ATOM		0 LY			24. 275	58. 217	1.00 40.67	B	Ŏ
ATON	10738	n me	T 616	94. 373	26.474	57.809	1.00 37.04	В	N
ATON		CA ME			26.744	58.948	1.00 36.91	В	C
ATON		CB ME			28.047	58. 738	1.00 36.80	В	C
ATOM		CG ME			27. 961	57.613	1.00 36.28	В	C
ATOM		SD ME			29. 532	57. 282	1.00 40.04	В	S
ATOM		CE ME			29. 023	56. 125	1.00 35.34	В	C
ATOM Atom		C ME O ME			26.817	60. 200	1.00 35.92	В	C
ATOM		N GL			27. 143 26. 514	60. 130 61. 343	1.00 35.52 1.00 33.40	B B	0 N
ATOM		CA GL			26. 505	62. 587	1.00 33.40	В	N C
ATOM		C GL			27. 783	63. 072	1.00 29.42	В	Ç .
ATOM		0 GL			27. 729	63. 689	1.00 30.60	В	ŏ
ATOM		N PH			28. 926	62. 797	1.00 26.74	B	Ň
ATOM		CA PH	E 618		30. 204	63. 271	1.00 25.54	B	Ĉ
ATOM		CB PH			31.118	63.636	1.00 26.06	В	C
ATOM		CG PH		95. 898	31.216	62.563	1.00 25.52	В	С
ATOM		CD1 PH		95. 763	32. 127	61. 523	1.00 25.78	В	C C C C
ATOM		CD2 PH		97.012	30. 385	62. 588	1.00 25.30	В	C
ATOM ATOM		CE1 PHI CE2 PHI		96. 726 97. 981	32. 214	60.518	1.00 26.10	В	C
ATOM		CZ PHI		97. 836	30. 459 31. 380	61.590 60.549	1.00 26.94 1.00 27.08	В	C
ATOM		C PHI		92. 706	30. 948	62.353	1.00 27.08	B B	C C
ATOM	10760	0 PHI		92. 319	32.079	62.644	1.00 24.00	В	0
ATOM		N VAI		92. 297	30. 313	61. 259	1.00 24.11	В	N
ATOM	10762	CA VAI		91.381	30. 947	60. 324	1.00 25.04	В	Ç
ATOM	10763	CB VAI		91.913	30.876	58.875	1.00 25.17	B	č
ATOM	10764	CG1 VAI		91.007	31.665	57.945	1.00 23.09	В	C
ATOM	10765	CG2 VAI		93. 326	31.415	58.817	1.00 26.33	В	C
ATOM	10766	C VAI		90. 004	30. 303	60. 371	1.00 25.53	В	С
ATOM		0 VAI		89. 873	29.083	60. 378	1.00 25.84	В	0
ATOM ATOM	10768	N ASI		88. 981	31.146	60.405	1.00 26.00	В	N
ATOM	10769 10770	CA ASI CB ASI		87. 601 86. 779	30. 701	60.449	1.00 26.41	В	C
ATOM	10771	CG ASI		85. 324	31.717 31.334	61.238 61.355	1.00 26.64 1.00 27.36	В	C .
ATOM	10772	OD1 ASE		84. 591	32.074	62.041	1.00 27.30	B B	C
ATOM	10773	OD2 ASE		84. 914	30. 306	60. 765	1.00 26.86	В	0 0
ATOM	10774	C ASI		87. 104	30.610	59.011	1.00 27.59	В	C
ATOM	10775	0 ASF	620	86. 687	31.610	58. 435	1.00 27.47	В	Ö
ATOM	10776	N ASN		87. 144	29.409	58. 438	1.00 29.06	В	Ň
ATOM	10777	CA ASN		86. 733	29. 213	57.053	1.00 30.04	B	Ċ
ATOM	10778	CB ASN		86. 925	27. 752	56.622	1.00 33.33	В	C
ATOM	10779	CG ASN	621	86. 022	26. 782	57. 377	1.00 36.94	В	C
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					BIC 4	, , ,			(Continued)
					FIG. 4-3	222			
ATOM	10829	CD2		627		49.646	1.00 11.41	В	C
ATOM	10830	CE2		627	• • • • • • • • • • • • • • • • • • • •	50. 500	1.00 10.99	B B	C C
ATOM	10831	CE3		627	••••	48. 806 50. 826	1.00 9.75 1.00 14.55	В	C
ATOM	10832	CD1		627		51. 208	1.00 14.35	В	N N
ATOM	10833	NE1 CZ2		627 627		50. 536	1.00 10.25	В	Č
ATOM	10834 10835	CZ3		627		48. 844	1.00 9.47	В	č
ATOM ATOM	10836	CH2		627		49. 702	1.00 8.43	B	č
ATOM	10837	C	TRP	627			·1.00 17.27	B	Č
ATOM	10838	0.	TRP	627		47. 732	1.00 16.96	В	0
ATOM	10839	Ň	GLY	628		46. 459	1.00 16.52	В	N
ATOM	10840	CA	GLY	628		45.675	1.00 16.52	В	C
ATOM	10841	C	GLY	628		44.975	1.00 17.44	В	С
ATOM	10842	0	GLY	628		44. 887	1.00 17.88	В	0
ATOM	10843	N	TRP	629		44. 479	1.00 15.93	В	N
ATOM	10844	CA	TRP	629		43. 781	1.00 15.93	В	C
ATOM	10845	CB	TRP	629		44. 552	1.00 13.57	В	C
ATOM	10846	CG	TRP	629		44. 341	1.00 14.96	В	C
MOTA	10847	· CD2		629		45. 360	1.00 13.15	В	C C
ATOM	10848	CE2		629		44. 712	1.00 13.17	B B	č
ATOM	10849	CE3		629		46. 758 43. 149	1.00 14.07 1.00 14.45	В	Č
ATOM	10850	CD1		629 629		43. 366	1.00 14.43	В	N
ATOM	10851 10852	NE1 CZ2		629		45. 414	1.00 13.59	В	Č
ATOM ATOM	10853	CZ3		629		47. 461	1.00 14.81	В	č
ATOM	10854		TRP	629		46. 782	1.00 15.16	B	Č
ATOM	10855	C	TRP	629		42. 399	1.00 17.34	B	Ċ
ATOM	10856	ŏ	TRP	629		42. 285	1.00 18.55	В	0
ATOM	10857	Ň	SER	630		41.354	1.00 17.70	В	N
ATOM	10858	CA	SER	630	91.309 48.430	39. 982	1.00 17.70	В	С
ATOM	10859	CB	SER	630	92.649 49.144	39.846	1.00 18.19	В	C
ATOM	10860	0G	SER	630		40. 404	1.00 24.67	В	0
ATOM	10861	C	SER	630	91.477 46.977	39. 563	1.00 17.40	В	C
ATOM	10862	0	SER	630	90. 501 46. 235	39. 469	1.00 18.69	В	0
ATOM	10863	N	TYR	631	92. 712 46. 565	39. 304	1.00 16.34	В	N
ATOM	10864	CA	TYR	631	92. 951 45. 192	38. 904	1.00 15.96	В	C
ATOM	10865	CB	TYR	631	94. 430 44. 973	38. 579	1.00 15.36	В	C
ATOM	10866	CG	TYR	631	94. 689 43. 709	37. 779	1.00 15.93	В	C
ATOM	10867		TYR	631	94. 626 42. 450	38. 380 37. 634	1.00 15.38 1.00 16.25	B B	C C
ATOM	10868		TYR	631	94.830 41.287 94.961 43.773	36. 409	1.00 15.25	В	C
ATOM	10869		TYR	631 631	94. 961 43. 773 95. 160 42. 620	35. 655	1.00 13.07	В	C
ATOM ATOM	10870 10871	CZ	TYR TYR	631	95. 092 41. 384	36. 270	1.00 15.96	В	C C C
ATOM	10872	OH	TYR	631	95. 264 40. 243	35. 525	1.00 14.59	В	ŏ
ATOM	10873	C	TYR	631	92. 499 44. 286	40.049	1.00 15.68	В	č
ATOM	10874	Õ	TYR	631	91.949 43.213	39. 824	1.00 16.42	В	ŏ
ATOM	10875	N	GLY	632	92.723 44.729	41. 281	1.00 15.56	B	N
ATOM	10876	CA	GLY	632		42. 429	1.00 14.43	B	С
ATOM	10877	C	GLY	632	90.777 43.807	42. 398	1.00 13.07	В	. C
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									(Continued)
					FIG.	4 - 223			(Continued)
			ar	200			1 00 10 00	n	0
ATOM	10878	0	GLY	632	90. 239 42.	771 42.777 855 41.946	1.00 12.09 1.00 12.57	B B	O N
ATOM	10879 10880	N CA	GLY GLY	$\begin{array}{c} 633 \\ 633 \end{array}$		800 41.846	1.00 12.31	В	Ċ
ATOM ATOM	10881	C	GLY	633		743 40.818	1.00 10.78	B	č
ATOM	10882	ŏ	GLY	633		956 40.986	1.00 9.26	B	0
ATOM	10883	N	TYR	634		729 39.734	1.00 11.33	В	N
ATOM	10884	ĊA	TYR	634		755 38.682	1.00 11.09	В	C
ATOM	10885	CB	TYR	634	89.860 42.		1.00 7.35	В	С
ATOM	10886	CG	TYR	634		899 36.526	1.00 8.04	В	С
ATOM	10887		TYR	634		162 36. 204	1.00 7.58	В	C
ATOM	10888		TYR	634		218 35.189	1.00 7.56	В	C
ATOM	10889		TYR	634		660 35.805	1.00 8.82	В	C
ATOM	10890		TYR	634		715 34.788	1.00 7.88	В	C
ATOM	10891	CZ	TYR	634		996 34.488	1.00 6.90	B B	C
ATOM	10892	OH	TYR	634		039 33. 504 358 39. 278	1.00 8.03 1.00 13.02	В	0 C
ATOM ATOM	10893 10894	C 0	TYR TYR	634 634		548 39. 222	1.00 13.02	В	Ö
ATOM	10895	N	VAL	635		091 39.858	1.00 14.38	В	Ň
ATOM	10896	CA	VAL	635		796 40.467	1.00 13.39	В	Ċ
ATOM	10897	CB	VAL	635		747 41.093	1.00 13.28	B	Č
ATOM	10898		VAL	635		467 41.923	1.00 13.06	В	Ċ
ATOM	10899		VAL	635	92.894 39.	782 39.999	1.00 8.09	В	C
ATOM	10900	С	VAL	635	89. 412 39.	443 41.533	1.00 13.35	В	C
ATOM	10901	0	VAL	635		320 41.563	1.00 15.02	В	0
ATOM	10902	N	THR	636		394 42.405	1.00 13.48	В	N
ATOM	10903	CA	THR	636		160 43.457	1.00 13.74	В	C
ATOM	10904	CB	THR	636		451 44. 260	1.00 15.19	В	C
ATOM	10905	OG1	THR	636		886 44.978	1.00 15.24	В	0
ATOM	10906	CG2	THR THR	636 636		188 45. 259 665 42. 862	1.00 13.51 1.00 14.57	B B	C C
ATOM ATOM	10907 10908	C 0	THR	636		750 43.395	1.00 14.57	В	0
ATOM	10909	N	SER	637		281 41.762	1.00 15.25	В	N N
ATOM	10910	CA	SER	637		905 41.112	1.00 15.03	В	Č
ATOM	10911	CB	SER	637		974 40. 102	1.00 16.88	B	č
ATOM	10912	0G	SER	637		158 40.766	1.00 18.07	B	Ō
ATOM	10913	Ċ	SER	637		558 40.420	1.00 16.54	В	Ċ
ATOM	10914	0	SER	637	84. 250 37.	773 40.487	1.00 17.87	В	0
ATOM	10915	N	MET	638		300 39.740	1.00 15.64	В	N
ATOM	10916	CA	MET	638		030 39.052	1.00 15.55	В	C
ATOM	10917	CB	MET	638		033 38. 272	1.00 15.97	В	C
ATOM	10918	CG	MET	638		959 37.067	1.00 17.38	В	C
ATOM	10919	SD	MET	638		422 35. 736	1.00 19.14	В	S
ATOM	10920	CE	MET	638		324 34.798	1.00 15.28	В	C
ATOM	10921	C	MET MET	638		913 40.093	1.00 17.56	B B	C
ATOM ATOM	10922 10923	0 N	VAL	638 639		807 39.843 199 41.260	1.00 17.45 1.00 16.50	В	O N
ATOM	10923	CA	VAL	639		207 42.317	1.00 10.30	В	C
ATOM	10925	CB	VAL	639		640 43.480	1.00 16.78	В	C
ATOM	10926		VAL	639		884 44.757	1.00 16.23	B	č
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	•				Ŧ	` T (G. 4-	224				(Con	tinued)
					1	1 (J. I	224					
ATOM	10927	CG2	VAL	639	89	. 495	35. 335	43. 139	1.00	14.45	В	С	
ATOM	10928	С	VAL	639		. 742	34.919	42.875		17.57	В	C	
ATOM	10929	0	VAL	639		. 387	33.760	43.081	1.00	18.52	В	0	
ATOM	10930	N	LEU	640		. 957	35.964	43. 124	1.00	16.90	В	N	
ATOM	10931	CA	LEU	640		. 618	35.766	43.661		17.42	В	С	
ATOM	10932		LEU	640		. 978	37. 098	44.032		17.45	В	С	
ATOM	10933		LEU	640		. 512	37.699	45.327		17.52	В	C	
ATOM	10934	CD1		640		. 743	38. 962	45.654		14.30	В	C	
ATOM	10935	CD2		640		. 378	36. 677	46.447		15.97	В	C	
ATOM	10936		LEU	640		. 713	35. 020	42.699		17.81	В	C	
ATOM	10937	0	LEU	640		. 821	34. 284	43.119		20.73	В	0	
ATOM	10938	N	GLY	641		. 952	35. 198	41.409		18.14	В	N	
ATOM	10939		GLY	641		. 135	34. 526	40.418		17.61	В	C	
ATOM	10940	C	GLY	641	84 99	. 758	33. 235	39. 936 38. 911		17.52 15.15	В	C	
ATOM ATOM	10941 10942	0 N	GLY SER	641 642		. 346 . 735	32. 697 32. 727	40. 683		17.53	B B	O N	
ATOM	10942	N CA	SER	642		. 419	31. 497	40. 003		19.98	В	C	
ATOM	10943	CB	SER	642		841	31. 479	40. 864		20.78	В	Č	
ATOM	10945	OG	SER	642		849	31.088	42. 226		21.56	В	ő	
ATOM	10946	C	SER	642		691	30. 239	40. 755		21.75	В	č	
ATOM	10947	Ŏ	SER	642		974	29. 147	40. 265		22.65	B	ŏ	
ATOM	10948	Ñ.	GLY	643		768	30. 395	41.701		22.05	B	Ň	
ATOM	10949		GLY	643		. 023	29. 258	42.210		22.58	B	C	
ATOM	10950	С	GLY	643		. 811	28.335	43.130		24.03	В	C	
ATOM	10951	0	GLY	643		460	27.162	43.271	1.00	26.05	В	0	
ATOM	10952	N	SER	644	83	. 859	28.849	43.772	1.00	22.41	В	N	
ATOM	10953	CA	SER	644		. 684	28.024	44.656		21.56	В	C	
ATOM	10954	CB	SER	644		. 065	28.657	44. 833		21.02	В	С	
ATOM	10955	0G	SER	644		. 992	29. 798	45.666		22.35	В	0	
ATOM	10956	C	SER	644		. 084	27. 773	46.037		21.06	В	C	
ATOM	10957	0	SER	644		451	26.807	46. 707		23. 51	В	0	
ATOM	10958	N	GLY	645		. 175	28. 643	46. 469		19.50	В	N	
ATOM	10959		GLY	645		. 561	28. 485	47. 774		16.85	В	C	
ATOM	10960	C	GLY	645		. 484	28. 868	48. 920		18.76	В	C	
ATOM	10961	O N	GLY VAL	645		. 111	28. 771	50.090		18. 32	В	0	
ATOM ATOM	10962 10963		VAL	646 646		691	29. 320 29. 695	48. 591 49. 612		18. 97 18. 18	В	N	
ATOM	10964	CB	VAL	646		. 009	29. 718	49.012		19. 50	B B	C C	
ATOM	10965	CG1		646		082	30. 202	50. 086		17.45	В	C	
ATOM	10966	CG2		646		471	28. 341	48. 516		17. 29	В	C	
ATOM	10967	C	VAL	646		433	31.051	50. 266		18. 24	В	C	
ATOM	10968	ŏ	VAL	646		860	31. 270	51.396		20. 76	В	Õ	
ATOM	10969	Ň	PHE	647		763	31.957	49. 561		16. 76	В	N	
ATOM	10970		PHE	647		525	33. 297	50. 082		16.60	В	Ċ	
ATOM	10971		PHE	647		066	34. 337	49. 094		16.44	В	č	
ATOM	10972		PHE	647		528	34. 204	48. 820		15. 63	B	č	
ATOM	10973	CD1		647		455	34. 941	49. 553		14. 72	B	Č	
ATOM	10974	CD2	PHE	647		985	33. 320	47.844		14.49	B	Č	
ATOM	10975	CE1	PHE	647		826	34.800	49. 317		16.66	В	Č	

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					FΙ	G. 4	225			(Co	ntinued)
ATOM	10976		PHE	647	88. 356			1.00 16.7		C	
ATOM	10977	CZ	PHE	647				1.00 13.3		C	
ATOM	10978	Ç	PHE	647	83.068			1.00 16.7		C	
ATOM	10979	0	PHE	647	82. 194		49. 551	1.00 17.3		0	
ATOM	10980	N	LYS	648	82. 819		51.515	1.00 16.7		N	
ATOM	10981	CA	LYS	648	81.466		51.905	1.00 19.6		C	
ATOM	10982	CB	LYS	648	81.369		53. 429	1.00 19.8		C C	
ATOM	10983 10984	CG CD	LYS LYS	648 648	80. 069 79. 876		53. 911 55. 393	1.00 21.9 1.00 23.1		C	
ATOM ATOM	10985	CE	LYS	648	78. 548		55.814	1.00 23.1		C	
ATOM	10986	NZ	LYS	648				1.00 24.3		N	
ATOM	10987	C	LYS	648				1.00 21.0		Č	
ATOM	10988	ŏ	LYS	648				1.00 20.2		ŏ	
ATOM	10989	Ň	CYS	649	81.954		51. 237	1.00 20.6		Ň	
ATOM	10990	CA	CYS	649	81.670		50. 711	1.00 21.9		C	
ATOM	10991	C	CYS	649	82. 928		50.134	1.00 22.7		C	
ATOM	10992	0	CYS	649	84.054		50.477	1.00 23.6	8 B	0	
ATOM	10993	CB	CYS	649	81.124	39.045	51.822	1.00 23.5		C	
ATOM	10994	SG	CYS	649	82. 287		53. 208	1.00 26.8		S	
ATOM	10995	N	GLY	650	82. 728		49. 267	1.00 20.1		N	
ATOM	10996	CA	GLY	650	83. 850		48.668	1.00 18.4		C	
ATOM	10997	C	GLY	650	83. 484		48. 308	1.00 18.0		C	
ATOM	10998	0	GLY	650	82. 308		48. 135	1.00 18.1		0	
ATOM ATOM	10999	N CA	ILE ILE	651 651	84. 490		48. 209	1.00 17.4		N	
ATOM	11000 11001	CB	ILE	651	84. 284 84. 632		47. 851 49. 014	1.00 15.9 1.00 15.4		C	
ATOM	11001		ILE	651	84. 386		48. 589	1.00 15.4		C	
ATOM	11002		ILE	651	83. 789		50. 242	1.00 15.8		Č	
ATOM	11004		ILE	651	84. 017		51.411	1.00 14.8		č	
ATOM	11005	C	ILE	651	85. 190		46. 679	1.00 16.4		č	
ATOM	11006	0	ILE	651	86. 404		46.754	1.00 16.6		ŏ	
ATOM	11007	N	ALA	652	84. 594		45.608	1.00 16.0		N	
ATOM	11008	CA	ALA	652	85. 330		44.413	1.00 15.1		C	
ATOM	11009	CB	ALA	652	84. 809		43. 214	1.00 16.3		C	
ATOM	11010	C	ALA	652	85. 190		44. 153	1.00 15.8		C	
ATOM	11011	0	ALA	652	84. 089		43.895	1.00 14.3		0	
ATOM	11012			653	86. 308			1.00 15.7			
	11013	CA		653	86. 298		43. 978	1.00 15.5		C	
ATOM ATOM	11014 11015	CB CG1	VAL	653 653	87.110		45.055	1.00 17.9		C	
ATOM	11015	CG2		653	87. 050 86. 566		44. 787	1.00 18.0		C	
ATOM	11017	C	VAL	653	86. 905		46. 446 42. 624	1.00 18.80 1.00 15.1		C	
ATOM	11018	ŏ	VAL	653	88. 071		42. 373	1.00 13.1		0	
ATOM	11019	Ň	ALA	654	86. 106		41.766	1.00 14.4		N	
ATOM	11020	CA	ALA	654	86. 532		40. 427	1.00 14.00		C	
ATOM	11021	CB	ALA	654	87. 424		40. 518	1.00 12.1		č	
ATOM	11022	C	ALA	654	87. 258		39. 700	1.00 12.48		č	
ATOM	11023	0	ALA	654	88. 364			1.00 13.1		ŏ	
ATOM	11024	N	PR0	655	86. 633			1.00 11.84		Ň	
					CHROTITUT		/DIN E 00	•			

					(Continued)
				FIG. 4-226	(Continuou)
ATOM .	11025	CD PRO	655	85. 273 47. 797 40. 088 1. 00 11. 50 B	С
ATOM ATOM	11025	CA PRO	655	87. 247 47. 003 38. 954 1. 00 11. 05 B	Č
ATOM	11027	CR PRO	655	86. 399 45. 841 39. 436 1. 00 11. 09 B	Č
ATOM	11028	CG PRO	655	85. 030 46. 451 39. 428 1. 00 8. 50 B	C
ATOM	11029	C PRO	655	87. 190 47. 102 37. 447 1. 00 10. 92 B	C
ATOM	11030	0 PRO	655	86. 383 47. 847 36. 896 1. 00 11. 41 B	0
ATOM	11031	n val	656	88.066 46.352 36.791 1.00 9.60 B	N
ATOM	11032	CA VAL	656	88. 052 46. 250 35. 345 1. 00 9. 08 B	C
ATOM	11033	CB VAL	656	89. 452 45. 888 34. 790 1. 00 7. 45 B	C
ATOM	11034	CG1 VAL	656	89.336 45.163 33.451 1.00 5.90 B	C
ATOM	11035	CG2 VAL	656	90. 249 47. 146 34. 601 1. 00 7. 63 B	C ,
ATOM	11036	C VAL	656	87.107 45.056 35.224 1.00 10.20 B	C
ATOM	11037	0 VAL	656	87. 157 44. 152 36. 058 1. 00 10. 59 B 86. 231 45. 038 34. 230 1. 00 11. 76 B	O N
ATOM	11038	N SER CA SER	657 657	86. 231 45. 038 34. 230 1. 00 11. 76 B 85. 313 43. 908 34. 115 1. 00 14. 03 B	C
ATOM ATOM	11039 11040	CA SER CB SER	657	83. 867 44. 375 34. 271 1. 00 13. 85 B	Č
ATOM	11040	OG SER	657	83. 495 45. 242 33. 218 1. 00 15. 07 B	ŏ
ATOM	11041	C SER	657	85. 456 43. 153 32. 812 1. 00 14. 66 B	č
ATOM	11043	0 SER	657	85. 191 41. 952 32. 743 1. 00 17. 18 B	Ö
ATOM	11044	N ARG	658	85. 887 43. 860 31. 781 1. 00 14. 15 B	N
ATOM	11045	CA ARG	658	86.050 43.277 30.459 1.00 13.24 B	C
ATOM	11046	CB ARG	658	84. 768 43. 532 29. 670 1. 00 14. 22 B	С
ATOM	11047	CG ARG	658	84. 763 43. 086 28. 231 1. 00 18. 57 B	C
ATOM	11048	CD ARG	658	83. 436 43. 470 27. 588 1. 00 19. 40 B	C
ATOM	11049	NE ARG	658	83. 475 43. 338 26. 138 1. 00 23. 11 B	N ·
ATOM	11050	CZ ARG	658	82. 868 42. 376 25. 454 1. 00 22. 54 B	C
ATOM	11051	NH1 ARG	658	82.167 41.445 26.088 1.00 21.95 B	N N
ATOM	11052	NH2 ARG	658	82. 955 42. 361 24. 131 1. 00 22. 77 B	N C
ATOM ATOM	11053 11054	C ARG O ARG	658 658	87. 242 44. 014 29. 857 1. 00 12. 76 B 87. 218 45. 239 29. 733 1. 00 11. 97 B	C 0
ATOM	11054	N TRP	659	88. 282 43. 283 29. 476 1. 00 11. 05 B	N N
ATOM	11056	CA TRP	659	89. 468 43. 942 28. 955 1. 00 12. 23 B	Č
ATOM	11057	CB TRP	659	90.578 42.918 28.777 1.00 11.99 B	
ATOM	11058	CG TRP	659	91.026 42.392 30.112 1.00 13.26 B	č
ATOM	11059	CD2 TRP	659	91.729 43.120 31.122 1.00 12.61 B	C C C
ATOM	11060	CE2 TRP	659	91. 848 42. 271 32. 242 1. 00 13. 22 B	Ċ
ATOM	11061	CE3 TRP	659	92. 268 44. 412 31. 193 1. 00 14. 19 B	C
ATOM	11062	CD1 TRP	659	90.759 41.163 30.644 1.00 13.17 B	C
ATOM	11063	NE1 TRP	659	91. 247 41. 083 31. 920 1. 00 13. 29 B	N
ATOM	11064	CZ2 TRP	659	92. 489 42. 670 33. 424 1. 00 13. 99 B	C
ATOM	11065	CZ3 TRP	659	92. 909 44. 810 32. 373 1. 00 13. 35 B	C
ATOM	11066	CH2 TRP	659	93. 011 43. 940 33. 468 1. 00 11. 92 B	C
ATOM	11067	C TRP	659	89. 338 44. 840 27. 730 1. 00 13. 23 B	C
ATOM	11068	O TRP	659	90.118 45.766 27.569 1.00 15.39 B	0 N
ATOM ATOM	11069 11070	N GLU CA GLU	660 660	88. 361 44. 595 26. 871 1. 00 14. 59 B 88. 181 45. 453 25. 708 1. 00 15. 33 B	N C
ATOM	11070	CA GLU	660	87. 147 44. 854 24. 743 1. 00 18. 10 B	C C
ATOM	11072	CG GLU	660	87. 572 43. 527 24. 130 1. 00 13. 10 B	C
ATOM	11073	CD GLU	660	86. 452 42. 829 23. 386 1. 00 25. 49 B	č
		020			•

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1.00 29.78

1.00 26.73

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O 97 (Continued)

0

0

В

				ric	7. 4 ⁻	221
ATOM	11074	OE1 GLU	660	86. 087	43. 278	22. 279
ATOM	11075	OE2 GLU	660		41.825	
ATOM	11076	C GLU	660	87.719	46.833	26.170

ATO! 1.00 14.88 C В ATOM **GLU** 87.661 47.769 25.375 11077 0 660 1.00 14.50 В 0 87. 371 86. 941 11078 ATOM 46.960 27.450 N TYR 661 1.00 14.66 В N 11079 48.258 ATOM CA TYR 661 27.977 1.00 15.13 В C **ATOM** 11080 85.988 48.119 CB TYR 661 29.168 1.00 15.73 В C 84.599 **ATOM** 11081 CG 47.597 28.872 TYR 661 1.00 19.12 В · C 47.053 29.898 C ATOM 11082 CD1 TYR 83.823 661 1.00 18.37 В 46. 548 82.553 **ATOM** 11083 CE1 TYR 661 29.653 1.00 19.84 В CD2 TYR ATOM 11084 84.061 47.629 C 661 27.581 1.00 19.07 В 11085 82.782 ATOM CE2 TYR 47.123 27.323 C 661 1.00 20.28 В ATOM 82.035 46.581 Ċ 11086 CZ TYR 661 28.367 1.00 20.80 B 11087 ATOM OH 80.785 TYR 661 46.046 28.142 1.00 20.60 В 0 ATOM 11088 88.146 C TYR 661 49.045 28.464 1.00 14.96 В C ATOM 11089 88.083 0 TYR 661 50.266 28.555 1.00 14.55 В 0 89.239 **ATOM** 11090 N TYR 662 48.355 28.789 1.00 14.46 В N 11091 **ATOM** CA TYR 662 90.411 49.060 29.289 1.00 15.14 В C ATOM 11092 91.225 CB TYR 662 48.182 30.240 1.00 13.98 В C 92.049 ATOM 11093 TYR CG 662 49.021 31.187 1.00 14.52 В C 93. 379 11094 ATOM CD1 TYR 48.699 662 31.468 1.00 14.22 В C ATOM 11095 CE1 TYR 94.168 49.531 662 32.255 1.00 11.31 C В ATOM 11096 CD2 TYR 91.522 50.194 662 31.734 1.00 13.44 C В MOTA 11097 CE2 TYR 92.297 51.030 1.00 13.70 662 32.520 C В ATOM 11098 CZ TYR 93.620 662 50.699 32.776 1.00 13.69 C В ATOM 11099 0H 94.395 TYR 662 51.549 33.532 1.00 12.84 0 В ATOM 11100 C TYR 91.309 49.615 662 28.182 1.00 15.44 R C ATOM 11101 0 91.095 49.337 TYR 662 26.996 1.00 15.06 В 0 ATOM 11102 N ASP 663 92.310 50.405 28.569 1.00 13.90 В N ATOM 11103 93. 192 CA **ASP** 663 51.026 27.588 1.00 13.58 В C ATOM 11104 CB **ASP** 93.961 663 52.192 28.238 1.00 13.61 C В ATOM 11105 CG **ASP** 663 95.093 51.741 29.152 1.00 14.10 C B ATOM 11106 OD1 ASP 663 95. 223 52.327 30.243 1.00 12.30 B 0 ATOM 11107 95.869 0D2 ASP 663 50.836 28.780 1.00 13.70 В 0 ATOM 11108 94.139 C ASP 663 50.076 26.850 1.00 13.21 В C ATOM 11109 0 ASP 663 94.565 49.045 27.378 1.00 13.05 В 0 ATOM 11110 N SER 664 94.453 50.444 25.612 1.00 13.86 В N 11111 **ATOM** CA SER 664 95.321 49.658 24.738 1.00 13.65 В C ATOM 11112 CB SER 664 95.464 50.364 23.394 1.00 14.44 В C ATOM 11113 0G SER 664 96.055 51.642 23.550 1.00 16.79 В 0 ATOM 11114 C SER 96.714 49.340 25.278 664 1.00 13.42 В C ATOM 11115 0 SER 97.066 664 48.176 25.438 1.00 12.83 В 0 ATOM 11116 N 25.559 VAL 665 97.503 50.371 1.00 12.98 В N ATOM 11117 CA VAL 665 98.865 50.158 26.041 1.00 15.86 В C ATOM 11118 CB VAL 665 99.547 51.496 26.427 1.00 14.66 В C ATOM 11119 CG1 VAL 665 101.023 Č 51.263 26.663 1.00 14.68 В ATOM 11120 CG2 VAL 665 99.354 1.00 15.28 52.519 25.327 В C ATOM 11121 C

> 48. 400 SUBSTITUTE SHEET (RULE 26)

49.169

27. 206

27. 242

1.00 15.25

1.00 15.22

C

0

В

B

99.020

99.972

VAL

VAL

ATOM

11122

0

665

665

				FIG	G. 4-	228			(Continued)
ATOM	11123		YR 666	98. 091	49. 184	28. 154	1.00 17.07	В	N
ATOM	11124		YR 666			29. 299	1.00 15.32	В	C
ATOM	11125 11126		YR 666 YR 666			30. 531 31. 751	1.00 13.28 1.00 12.79	B B	C
ATOM ATOM	11120	CD1 T				31. 845	1.00 12.79	В	C
ATOM	11128	CE1 T				32.964	1.00 12.21	В	č
ATOM	11129	CD2 T				32. 809	1.00 12.83	В	Č
ATOM	11130	CE2 T				33. 928	1.00 11.79	B	Č
ATOM	11131		YR 666			34.005	1.00 13.90	В	С
ATOM	11132	OH T	YR 666	97. 471	45. 531	35. 131	1.00 12.51	В	0
ATOM	11133		YR 666			29. 023	1.00 15.26	В	C
ATOM	11134		YR 666			29. 399	1.00 18.30	В	0
ATOM	11135		HR 667		46. 912	28. 365	1.00 14.70	В	N
ATOM	11136		HR 667			28. 097	1.00 13.70	В	C
ATOM	11137		HR 667			27. 656 28. 635	1.00 12.07 1.00 11.17	B B	C
ATOM ATOM	11138 11139		HR 667 HR 667		40. 730	27. 533	1.00 11.17	В	C 0
ATOM	11140		HR 667			27.067	1.00 15.21	В	Č
ATOM	11141		HR 667			27. 323	1.00 16.16	В	ŏ
ATOM	11142		LU 668		45. 372	25. 906	1.00 16.99	B	Ň
ATOM	11143		LU 668		44.672	24. 823	1.00 16.90	$\tilde{\mathtt{B}}$	Č
ATOM	11144		LU 668		45.612	23.625	1.00 17.50	B	Ċ
ATOM	11145		LU 668		45.808	22.867	1.00 21.31	В	С
ATOM	11146		LU 668		46.928	21.850	1.00 22.06	В	C
ATOM	11147	OE1 G				21.123	1.00 25.39	В	0
ATOM	11148	OE2 G			47.679	21.767	1.00 22.03	В	0
ATOM	11149		LU 668		44. 127	25. 247	1.00 17.77	В	C
ATOM	11150		LU 668		43.079	24. 766	1.00 19.28	В	0
ATOM ATOM	11151 11152		RG 669 RG 669		44. 827 44. 392	26. 158 26. 640	1.00 17.62 1.00 17.00	В	N
ATOM	11152		RG 669	100. 721 101. 199	44. 392 45. 291	27. 785	1.00 17.00	B B	C C
ATOM	11154		RG 669	102. 498	44. 828	28. 451	1.00 15.11	В	C
ATOM	11155		RG 669	102. 878		29. 583	1.00 15.35	B	Č
ATOM	11156		RG 669	102. 914	47. 149	29. 122	1.00 16.25	B	Ň
ATOM	11157		RG 669	102.549	48.196	29.856	1.00 16.96	B	Ĉ
ATOM	11158		RG 669	102.115	48.023	31.101	1.00 16.86	В	N
ATOM	11159	NH2 Al		102.602	49.417	29. 340	1.00 14.86	В	N
ATOM	11160		RG 669		42.960	27. 140	1.00 17.70	В	C
ATOM	11161		RG 669	101. 523	42.141	26.899	1.00 17.72	В	0
ATOM	11162		YR 670	99. 539	42.655	27. 825	1.00 17.60	В	N
ATOM	11163		YR 670	99.357	41.333	28. 385	1.00 16.56	В	C
ATOM ATOM	11164 11165		YR 670 YR 670	98. 823 99. 571	41.465 42.491	29. 810 30. 631	1.00 15.82 1.00 15.47	B	C
ATOM	11166	CD1 T		98. 978	43. 706	30. 973	1.00 15.47	B B	C C
ATOM	11167	CE1 T		99. 680	44. 676	31.676	1.00 14.00	В	C
ATOM	11168	CD2 T		100. 894	42. 268	31.024	1.00 15.93	В	Č
ATOM	11169	CE2 TY		101.608	43. 232	31. 732	1.00 15.78	В	č
ATOM	11170		TR 670	100. 998	44. 433	32.051	1.00 15.30	В	č
ATOM	11171		YR 670	101.713	45.403	32.714	1.00 15.22	B	Ŏ

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(Continued)

					FI	G. 4-	2 2 9			Continue
ATOM	11172	C	TYR	670	98. 435		27. 578	1.00 17.87	В	C
ATOM	11173	0	TYR	670	98. 637		27. 508	1.00 18.02	В	0
ATOM	11174	N	MET	671	97. 435		26. 948	1.00 18.57	В	N
ATOM	11175	CA	MET	671	96. 452		26. 199	1.00 19.04	В	C
ATOM	11176	CB	MET	671	95. 063		26. 482	1.00 21.47	В	C
ATOM	11177	CG	MET	671	94. 604		27. 919	1.00 21.74	В	C
ATOM	11178	SD	MET	671	94. 228		28. 277	1.00 28.61	В	S
ATOM	11179	CE	MET	671	92. 570		27. 582	1.00 23.84	В	C
ATOM	11180	C	MET	671	96. 640		24.692	1.00 19.95	B B	0
ATOM	11181	0	MET	671	96. 121		24. 075	1.00 20.85 1.00 20.28	В	N
ATOM	11182	N	GLY	672	97. 380		24. 094	1.00 20.28	В	C
ATOM	11183	CA	GLY GLY	672 672	97. 540 96. 354		22.654 22.068	1.00 19.00	В	C
ATOM	11184	C	GLY	672	90. 334 95. 746		22.755	1.00 21.12	В	0
ATOM ATOM	11185 11186	O N	LEU	673	96. 009		20. 814	1.00 21.18	В	N N
ATOM	11187	CA	LEU	673	94. 884		20. 186	1.00 21.00	В	C
ATOM	11188	CB	LEU	673	95. 204		18. 732	1.00 22.03	В	Ç.
ATOM	11189	CG	LEU	673	96. 287		18. 507	1.00 24.89	В	Č
ATOM	11190		LEU	673	96. 518		17. 023	1.00 23.45	В	Ç.
ATOM	11191		LEU	673	95. 846		19. 150	1.00 27.67	В	č
ATOM	11192	C	LEU	673	93. 616		20. 243	1.00 21.68	B	č
ATOM	11193	ŏ	LEU	673	93. 647		20.076	1.00 21.49	B	ŏ
ATOM	11194	Ň	PR0	674	92. 475			1.00 21.61	B	N
ATOM	11195	CD	PRO	674	92. 342		20. 830	1.00 20.79	B	Ċ
ATOM	11196	CA	PRO	674	91. 180		20. 571	1.00 20.99	B	Č
ATOM	11197	CB	PR0	674	90. 365		21.420	1.00 19.09	B	C C C
ATOM	11198	CG	PR0	674	90. 845		20.941	1.00 18.24	В	Č
ATOM	11199	С	PR0	674	90. 589		19.183	1.00 21.53	В	Ċ
ATOM	11200	0	PR0	674	89.470		18.884	1.00 20.30	В	0
ATOM	11201	N	THR	675	91.378	40. 505	18.335	1.00 23.61	В	N
ATOM	11202	CA	THR	675	90. 973	40.176	16.975	1.00 23.43	В	C
ATOM	11203	CB	THR	675	92. 045		15.957	1.00 22.99	В	C
ATOM	11204	0G1			93. 221		16.200	1.00 24.15	В	0
ATOM	11205		THR	675	92. 386		16.062	1.00 21.26	В	С
ATOM	11206	C	THR	675	90. 825		16.931	1.00 25.46	В	С
ATOM	11207	0	THR	675	91.424		17. 736	1.00 25.82	В	0
ATOM	11208	N	PR0	676	90. 023		15.991	1.00 26.60	В	N
	11209							1.00 25.76	В	C
ATOM	11210	CA	PR0	676	89. 823	36. 714	15.877	1.00 26.64	В	C
ATOM	11211	CB	PRO	676	88. 860		14. 702	1.00 25.84	В	C
ATOM	11212	CG	PRO	676	88.066	37. 859	14.801	1.00 24.99	В	Č .
ATOM	11213	Č	PRO	676	91. 135	35. 967	15.630	1.00 28.63	В	C
ATOM	11214	0	PR0	676	91.347	34. 875	16. 160	1.00 28.85	В	0
ATOM	11215	N	GLU	677	92. 021	36. 557	14. 834	1.00 30.55	В	N.
ATOM	11216	CA	GLU	677	93. 286	35. 905	14. 534	1.00 31.94	В	C
ATOM	11217	CB	GLU	677	93. 772	36. 290	13: 135	1.00 35.44	В	C
ATOM	11218	CC	GLU	677	94. 177	35. 077	12. 294	1.00 41.76	В	C
ATOM	11219	CD	GLU	677	92. 984	34. 204	11.897	1.00 46.15	В	C
ATOM	11220	0E1	GLU	677	92. 234	34. 610	10. 980	1.00 49.52	В	0

ATOM 11221 0E2 GLU 677 92.789 33.121 12.503 1.00 46.47 B 0 ATOM 11223 0 GLU 677 94.382 36.174 15.563 1.00 31.51 B C ATOM 11223 0 GLU 677 94.382 36.174 15.563 1.00 31.51 B 0 ATOM 11224 N ASP 678 94.003 36.680 16.730 1.00 29.04 B N ATOM 11225 CA ASP 678 95.005 36.896 17.756 1.00 26.71 B C ATOM 11226 CB ASP 678 95.005 36.896 17.756 1.00 26.71 B C ATOM 11226 CB ASP 678 95.509 38.374 17.917 1.00 25.30 B C ATOM 11226 CB ASP 678 95.509 38.586 18.902 1.00 26.53 B C ATOM 11229 002 ASP 678 95.500 33.586 18.902 1.00 26.53 B C ATOM 11229 002 ASP 678 95.600 37.612 19.579 1.00 24.47 B O ATOM 11230 C ASP 678 94.586 36.325 19.098 1.00 25.24 B C ATOM 11230 ASP 678 94.586 36.325 19.098 1.00 26.23 B O ATOM 11230 ASP 678 94.586 36.325 19.098 1.00 26.23 B O ATOM 11233 C ASN 679 93.814 37.082 19.871 1.00 24.14 B N ATOM 11233 CA ASN 679 93.814 37.082 19.871 1.00 24.14 B N ATOM 11233 CA ASN 679 94.456 37.089 21.100 10.00 27.00 B C ATOM 11235 CG ASN 679 94.456 37.089 21.100 11.00 22.73 B C ATOM 11235 CG ASN 679 94.456 37.089 21.100 10.00 22.05 B C ATOM 11235 CG ASN 679 94.644 36.880 24.592 1.00 21.44 B O ATOM 11237 DASN 679 94.690 35.037 23.448 1.00 22.30 B N ATOM 11238 C ASN 679 94.691 35.037 23.448 1.00 22.30 B N ATOM 11238 C ASN 679 94.691 35.037 23.448 1.00 22.30 B N ATOM 11238 C ASN 679 94.692 35.037 23.448 1.00 22.30 B N ATOM 11238 C ASN 679 94.693 35.037 23.448 1.00 22.30 B N ATOM 11238 C ASN 679 94.593 35.037 23.448 1.00 22.30 B N ATOM 11234 CB LEU 680 88.993 37.967 19.617 1.00 21.56 B O ATOM 11240 N LEU 680 91.53 37.316 20.619 1.00 22.05 B C ATOM 11240 N LEU 680 88.993 37.967 19.617 1.00 20.94 B C ATOM 11244 CD LEU 680 88.993 37.967 19.617 1.00 22.05 B C ATOM 11244 CD LEU 680 88.993 37.967 19.617 1.00 22.05 B C ATOM 11244 CD LEU 680 88.993 37.967 19.617 1.00 22.95 B N ATOM 11246 C LEU 680 88.993 37.967 19.617 1.00 22.96 B N ATOM 11246 C LEU 680 88.993 37.967 19.617 1.00 22.95 B N ATOM 11246 C LEU 680 88.993 37.967 19.617 1.00 22.96 B C ATOM 11246 C LEU 680 88.993 37.967 19.617 1.00 22.96 B C ATOM 11246 C LEU 680 88.993 37.967			(Continued)
ATOM 11222 C GLU 677 94.382 36.174 15.563 1.00 31.51 B C ATOM 11224 N ASP 678 94.003 36.680 16.730 1.00 29.04 B N ATOM 11224 N ASP 678 94.003 36.680 16.730 1.00 29.04 B N ATOM 11225 CA ASP 678 94.003 38.5680 16.730 1.00 29.04 B N ATOM 11226 CB ASP 678 95.005 36.896 17.756 1.00 26.71 B C ATOM 11227 CG ASP 678 95.509 38.586 18.902 1.00 26.53 B C ATOM 11228 0D1 ASP 678 97.004 39.721 19.008 1.00 29.18 B O ATOM 11229 0D2 ASP 678 96.500 38.586 18.902 1.00 26.53 B C ATOM 11229 0D2 ASP 678 96.500 38.586 18.902 1.00 24.47 B O ATOM 11230 C ASP 678 94.586 36.325 19.908 1.00 25.24 B C ATOM 11231 0 ASP 678 94.586 36.325 19.908 1.00 25.24 B C ATOM 11232 N ASN 679 93.418 36.608 21.186 1.00 26.23 B O ATOM 11231 C ASP 678 94.456 37.082 19.871 1.00 24.14 B N ATOM 11234 CB ASN 679 93.418 36.608 21.186 1.00 22.47 B C ATOM 11235 CG ASN 679 94.456 37.089 22.217 1.00 23.05 B C ATOM 11237 ADD ASN 679 94.659 35.037 23.448 1.00 22.30 B C ATOM 11237 ADD ASN 679 94.659 35.037 23.448 1.00 22.50 B C ATOM 11238 C ASN 679 94.659 35.037 23.448 1.00 22.50 B C ATOM 11237 ND2 ASN 679 94.659 35.037 23.448 1.00 22.50 B C ATOM 11238 C ASN 679 94.659 35.037 23.448 1.00 22.50 B C ATOM 11238 C ASN 679 94.059 35.037 23.448 1.00 22.50 B C ATOM 11238 C ASN 679 94.059 35.037 23.448 1.00 22.50 B C ATOM 11237 ND2 ASN 679 94.059 35.037 23.448 1.00 22.50 B C ATOM 11240 N LEU 680 88.783 37.750 20.913 1.00 22.96 B N ATOM 11241 C B LEU 680 88.783 37.967 19.617 1.00 20.94 B C ATOM 11244 CD LEU 680 88.783 37.967 19.617 1.00 20.94 B C ATOM 11244 CD LEU 680 88.993 37.967 19.617 1.00 20.94 B C ATOM 11244 CD LEU 680 88.993 37.967 19.617 1.00 20.94 B C ATOM 11249 C ASP 681 88.502 34.469 22.317 1.00 22.36 B C ATOM 11249 C ASP 681 88.502 34.469 22.317 1.00 22.96 B N ATOM 11249 C ASP 681 88.502 34.469 22.317 1.00 22.96 B N ATOM 11249 C ASP 681 88.502 34.469 22.317 1.00 22.96 B N ATOM 11245 CD ASP 681 88.502 34.469 22.317 1.00 22.96 B N ATOM 11245 CD ASP 681 88.502 34.692 20.90 33.408 20.90 33.90 1.00 21.18 B C ATOM 11250 C ASP 681 88.502 34.693 25.805 1.00 22.95 B N ATOM 1		FIG. 4-230	(Conumaca)
ATOM 11222 C GLU 677 94.382 36.174 15.563 1.00 31.51 B C ATOM 11224 N ASP 678 94.003 36.680 16.730 1.00 29.04 B N ATOM 11224 N ASP 678 94.003 36.680 16.730 1.00 29.04 B N ATOM 11225 CA ASP 678 95.005 36.896 17.756 1.00 26.71 B C ATOM 11227 CG ASP 678 95.005 38.896 18.705 1.00 26.71 B C ATOM 11227 CG ASP 678 95.505 38.374 17.917 1.00 25.30 B C ATOM 11228 0D1 ASP 678 97.004 39.721 19.008 1.00 29.18 B O ATOM 11229 0D2 ASP 678 96.500 38.586 18.902 1.00 26.53 B C ATOM 11229 0D2 ASP 678 96.500 38.586 18.902 1.00 26.53 B C ATOM 11229 0D2 ASP 678 96.500 38.586 18.902 1.00 24.47 B O ATOM 11230 C ASP 678 94.586 36.325 19.908 1.00 25.24 B C ATOM 11231 O ASP 678 94.586 36.325 19.908 1.00 25.24 B C ATOM 11232 N ASN 679 93.418 36.608 21.186 1.00 26.23 B O ATOM 11231 CA ASN 679 93.418 36.608 21.186 1.00 22.47 B C ATOM 11232 CA ASN 679 93.418 36.608 21.186 1.00 22.47 B C ATOM 11234 CB ASN 679 94.456 37.089 22.217 1.00 23.05 B C ATOM 11235 CG ASN 679 94.456 37.089 22.217 1.00 23.05 B C ATOM 11236 CD ASN 679 94.659 35.037 23.448 1.00 22.50 B N ATOM 11237 ND2 ASN 679 94.699 35.037 23.448 1.00 22.50 B N ATOM 11238 CD ASN 679 94.699 35.037 23.448 1.00 22.50 B N ATOM 11238 CD ASN 679 94.059 35.037 23.448 1.00 22.50 B N ATOM 11239 CD ASN 679 94.059 35.037 23.448 1.00 22.50 B N ATOM 11239 CD ASN 679 91.727 37.174 22.785 1.00 21.56 B C ATOM 11240 N LEU 680 88.793 37.967 19.617 1.00 20.94 B C ATOM 11244 CD LEU 680 88.993 37.967 19.617 1.00 20.94 B C ATOM 11244 CD LEU 680 88.993 37.967 19.617 1.00 20.94 B C ATOM 11244 CD LEU 680 88.993 37.967 19.617 1.00 20.94 B C ATOM 11244 CD LEU 680 88.993 37.967 19.617 1.00 20.94 B C ATOM 11240 CD ASP 681 88.502 34.469 22.311 1.00 24.77 B C ATOM 11247 CD LEU 680 88.993 37.967 19.617 1.00 20.98 B C ATOM 11249 CD ASP 681 88.502 34.692 20.95 1.00 22.86 B N ATOM 11249 CD ASP 681 88.502 34.692 20.95 1.00 22.86 B C ATOM 11240 CD ASP 681 88.502 34.692 20.95 1.00 22.86 B C ATOM 11250 CD ASP 681 88.502 34.692 20.95 1.00 22.86 B N ATOM 11250 CD ASP 681 88.502 34.693 25.872 10.00 22.95 B C ATOM 11250 CD ASP 681	ATOM 11221 OR2 GLJI 677	92.789 33.121 12.503 1.00 46.47	В 0
ATOM 11223 0 CLU 677 95.565 35.938 15.305 1.00 31.18 B O ATOM 11224 N ASP 678 94.003 36.680 16.730 1.00 29.04 B N ATOM 11225 CA ASP 678 95.005 36.896 17.756 1.00 26.71 B C ATOM 11226 CB ASP 678 95.059 38.374 17.917 1.00 25.30 B C ATOM 11227 CC ASP 678 95.509 38.586 18.902 1.00 26.53 B C ATOM 11228 ODI ASP 678 96.500 38.586 18.902 1.00 26.53 B C ATOM 11229 ODZ ASP 678 96.500 38.586 18.902 1.00 26.53 B C ATOM 11223 OD ASP 678 96.500 38.586 18.902 1.00 24.47 B O ATOM 11230 C ASP 678 94.586 36.325 19.098 1.00 25.24 B C ATOM 11231 O ASP 678 94.586 36.325 19.098 1.00 25.24 B C ATOM 11232 N ASN 679 93.418 36.608 21.186 1.00 22.47 B C ATOM 11233 CA ASN 679 93.418 36.608 21.186 1.00 22.47 B C ATOM 11235 CO ASP 679 94.456 37.089 22.217 1.00 24.14 B N ATOM 11235 CO ASP 679 94.456 37.089 22.217 1.00 23.05 B C ATOM 11235 CO ASN 679 94.456 37.089 22.217 1.00 23.05 B C ATOM 11235 CO ASN 679 94.456 37.089 22.217 1.00 23.05 B C ATOM 11235 CO ASN 679 94.456 37.089 22.217 1.00 23.05 B C ATOM 11235 CO ASN 679 94.659 35.037 23.448 1.00 22.50 B C ATOM 11235 CO ASN 679 94.699 35.037 23.448 1.00 22.50 B C ATOM 11235 CO ASN 679 94.059 35.037 23.448 1.00 22.50 B C ATOM 11235 CO ASN 679 94.059 35.037 23.448 1.00 22.50 B C ATOM 11235 C ASN 679 94.059 35.037 23.448 1.00 22.30 B N ATOM 11235 C ASN 679 94.059 35.037 23.448 1.00 22.30 B N ATOM 11241 CA LEU 680 89.783 37.750 20.913 1.00 22.95 B C ATOM 11241 CA LEU 680 89.783 37.316 20.619 1.00 22.95 B C ATOM 11241 CA LEU 680 89.783 37.350 20.913 1.00 22.05 B C ATOM 11241 CA LEU 680 89.783 37.750 20.913 1.00 22.95 B C ATOM 11241 CA LEU 680 89.783 37.350 20.913 1.00 22.95 B C ATOM 11241 CA LEU 680 89.913 37.950 20.913 1.00 22.95 B C ATOM 11241 CA LEU 680 89.913 37.950 20.913 1.00 22.95 B C ATOM 11241 CA LEU 680 89.913 37.950 20.913 1.00 22.95 B C ATOM 11245 CD 2 LEU 680 88.993 37.957 19.617 1.00 24.77 B C ATOM 11245 CD 2 LEU 680 88.993 37.957 19.617 1.00 22.95 B C ATOM 11245 CD 2 LEU 680 88.993 37.957 19.617 1.00 22.95 B C ATOM 11245 CD ASP 681 88.910 33.448 21.990 1.00 22.75 B C ATOM 11245 CD A			
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ATOM 11268 CB TYR 683 89.226 39.646 24.542 1.00 16.55 B C			
ATOM LIZON OF TRE DAY AND	ATOM 11269 CG TYR 683	90. 419 40. 574 24. 472 1. 00 16. 85	B C

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ATOM 11318 CA

MET

689

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(Continued) FIG. 4-231 23.877 1.00 16.29 91.616 40.172 C 11270 CD1 TYR 683 ATOM 92.700 C 23.786 1.00 16.38 41.040 ATOM 11271 CE1 TYR 683 В C 90.345 41.871 24.980 1.00 16.79 B 11272 CD2 TYR 683 ATOM 24.893 CE2 TYR 91.430 42.748 1.00 14.60 В 11273 ATOM 683 C 92.598 24.295 1.00 15.79 42.326 В ATOM 11274 CZ TYR 683 24.192 0 93.663 43.193 1.00 16.43 **ATOM** 11275 OH TYR 683 C 87.793 38.437 26.150 1.00 21.02 В **ATOM** 11276 C TYR 683 87.355 38.955 27.174 1.00 20.95 В 0 **ATOM** 11277 0 TYR 683 87.071 37.644 1.00 22.94 25.367 B N ATOM 11278 N ARG 684 ATOM 11279 85.667 37.349 25.634 1.00 24.36 В C CA ARG 684 Č 11280 84.992 36.871 24.344 1.00 24.11 В ATOM CB ARG 684 84.996 37.908 23.234 1.00 25.07 C В ATOM 11281 CG ARG 684 84.197 1.00 25.30 C 39.132 23.639 В ATOM 11282 CD ARG 684 11283 84.453 40.275 22.767 1.00 27.33 N ATOM NE ARG 684 В 84.126 ATOM 11284 ARG 40.344 21.480 1.00 27.26 В C CZ 684 83. 518 84. 409 11285 39.327 20.880 1.00 27.78 **ATOM** ARG В N NH1 684 11286 ARG 41.443 20.794 1.00 26.25 ATOM NH2 684 В N **ATOM** 11287 ARG 85.401 36.340 26.745 1.00 24.46 В C C 684 36.239 **ATOM** 11288 0 ARG 84.275 27.231 1.00 26.21 В 0 684 35.591 27.148 11289 N 1.00 24.53 ATOM ASN 685 86.421 В N 86.243 34.593 1.00 23.44 ATOM 11290 CA ASN 685 28.201 B C ATOM 11291 86.959 33.294 27.823 1.00 26.13 C CB ASN 685 В ATOM 11292 ASN 86.132 32.430 26.904 1.00 33.00 C CG В 685 85.076 31.924 1.00 35.72 ATOM 11293 OD1 ASN 27.296 685 В 0 86.594 32.260 ATOM 11294 ND2 ASN 685 25.667 1.00 36.03 В N 11295 86.716 **ATOM** C ASN 685 35.043 29.575 1.00 20.60 В C 86.472 1.00 20.98 11296 ATOM 0 ASN 685 34.361 30.566 В 0 87.382 ATOM 11297 N SER 686 36.186 29.644 1.00 16.28 В N ATOM 11298 CA SER 686 87.887 36.666 30.918 1.00 16.33 В C 11299 89.360 ATOM CB SER 686 37.063 30.773 1.00 17.18 C В 89. 530 87. 089 11300 ATOM SER 38.050 29.768 0G 686 1.00 17.94 В 0 ATOM 11301 37.837 C SER 686 31.486 1.00 15.71 В C ATOM 11302 87.625 38.667 32.221 1.00 13.91 0 SER 686 0 В ATOM 11303 85.807 37.905 31.155 1.00 14.37 N THR 687 В N 11304 84.989 38.992 ATOM CA THR 31.655 1.00 15.19 687 В C 83.899 ATOM 11305 CB THR 687 39.401 30.639 1.00 16.80 C В ATOM 11306 82.915 38.362 OG1 THR 687 30.537 1.00 18.14 В 0 ATOM 11307 CG2 THR 84.519 39.657 29.265 1.00 16.92 687 R C 84. 309 **ATOM** 11308 C THR 687 38.605 32.957 1.00 14.86 В C **ATOM** 11309 84. 153 0 THR 687 37.425 33.264 1.00 13.79 B 0 83. 910 11310 33.717 **ATOM** N VAL 688 39.616 1.00 14.71 N В ATOM 11311 CA VAL 688 83. 224 39.411 34.977 1.00 14.27 C В **ATOM** 11312 CB VAL 688 83. 239 40.691 35.824 1.00 15.67 C В 82.476 ATOM 11313 CG1 VAL 688 40.464 37.130 1.00 15.43 В C ATOM 11314 CG2 VAL 688 84.687 41.115 36.100 1.00 18.49 В C ATOM 11315 C VAL 688 81.777 39.048 34.687 1.00 14.74 В C ATOM 11316 0 VAL 688 81.196 38.188 35.350 1.00 15.40 0 В ATOM 11317 N MET 689 81.209 39.710 33.682 1.00 13.94 N

SUBSTITUTE SHEET (RULE 26)

33. 283

1.00 14.18

79.826 39.496

					770 4 000		(Continued)
					FIG. 4-232		
ATOM	11319	CB	MET	689	79.519 40.287 32.010 1.00 14.10	В	С
ATOM	11320	CG	MET	689	79. 359 41. 793 32. 217 1. 00 18. 18	В	C
ATOM	11321	SD	MET	689	80. 817 42. 684 32. 849 1. 00 21. 67	В	S
ATOM ATOM	11322 11323	CE C	MET MET	689 689	81. 693 43. 067 31. 308 1. 00 19. 11 79. 429 38. 040 33. 080 1. 00 13. 66	B B	C C
ATOM	11323	Ö	MET	689	78. 398 37. 597 33. 586 1. 00 14. 01	В	Ö
ATOM	11325	Ň	SER	690	80. 246 37. 290 32. 356 1. 00 14. 32	В	Ň
ATOM	11326	CA	SER	690	79. 939 35. 887 32. 087 1. 00 16. 68	B	C
ATOM	11327	CB	SER	690	81.018 35.259 31.199 1.00 18.28	В	C
ATOM	11328	0G	SER	690	82. 225 35. 062 31. 923 1. 00 23. 11	В	0
ATOM	11329	C	SER	690	79. 771 35. 019 33. 328 1. 00 15. 55	В	C
ATOM ATOM	11330 11331	O N	SER ARG	690 691	79. 212 33. 927 33. 234 1. 00 16. 21 80. 238 35. 502 34. 478 1. 00 14. 35	B B	O N
ATOM	11332	CA	ARG	691	80. 155 34. 741 35. 727 1. 00 15. 38	В	C
ATOM	11333	CB	ARG	691	81. 491 34. 821 36. 478 1. 00 16. 76	B	č
ATOM	11334	CG	ARG	691	82.697 34.414 35.652 1.00 19.96	В	C
ATOM	11335	CD	ARG	691	83. 972 34. 339 36. 483 1. 00 21. 36	В	C
ATOM	11336	NE	ARG	691	85.061 33.725 35.726 1.00 23.56	В	N
ATOM ATOM	11337 11338	CZ NH1	ARG ARG	691 691	86. 196 33. 274 36. 256 1. 00 26. 24 86. 418 33. 358 37. 567 1. 00 23. 55	В	C
ATOM	11339		ARG	691	87. 114 32. 728 35. 468 1. 00 26. 33	B B	N N
ATOM	11340	C	ARG	691	79.049 35.187 36.679 1.00 15.48	В	Č
ATOM	11341	Õ	ARG	691	78. 986 34. 713 37. 817 1. 00 14. 38	B	Ö
ATOM	11342	N	ALA	692	78. 178 36. 081 36. 220 1. 00 14. 78	В	N
ATOM	11343	CA	ALA	692	77.111 36.618 37.064 1.00 16.42	В	C
MOTA	11344	CB	ALA	692	76. 105 37. 383 36. 198 1. 00 16. 75	В	C
ATOM ATOM	11345 11346	C 0	ALA ALA	692 692	76. 375 35. 624 37. 977 1. 00 17. 17 76. 331 35. 814 39. 191 1. 00 16. 75	В	C
ATOM	11340	N	GLU	693	75. 803 34. 571 37. 404 1. 00 19. 44	B B	O N
ATOM	11348	CA	GLU	693	75. 062 33. 589 38. 191 1. 00 22. 16	В	Č
ATOM	11349	CB	GLU	693	74. 570 32. 443 37. 299 1. 00 26. 71	B	Č
ATOM	11350	CG	GLU	693	73. 251 32. 745 36. 598 1. 00 33. 79	В	C
ATOM	11351	CD	GLU	693	73.017 31.873 35.379 1.00 38.47	В	C
ATOM	11352 11353	0E1	GLU	693	72. 984 30. 632 35. 531 1. 00 40. 41	В	0
ATOM ATOM	11354	C	GLU GLU	693 693	72. 870 32. 433 34. 266 1. 00 41. 15 75. 827 33. 022 39. 369 1. 00 22. 08	B B	0 C
ATOM	11355	Ö	GLU	693	75. 244 32. 761 40. 418 1. 00 24. 44	В	0
ATOM	11356	Ň	ASN	694	77. 127 32. 824 39. 215 1. 00 21. 66	В	N
ATOM	11357	CA	ASN	694	77. 907 32. 282 40. 320 1. 00 22. 61	B	č
ATOM	11358	CB	ASN	694	79. 324 31. 924 39. 861 1. 00 20. 93	В	C
ATOM	11359	CG	ASN	694	79. 359 30. 654 39. 048 1. 00 19. 32	В	Ç
ATOM	11360		ASN	694	80. 284 30. 420 38. 278 1. 00 19. 68	В	0
ATOM ATOM	11361 11362	C	ASN ASN	694 694	78. 348 29. 818 39. 224 1. 00 18. 34 77. 975 33. 234 41. 500 1. 00 22. 99	В	N .
ATOM	11363	Ö	ASN	694	78.650 32.946 42.479 1.00 25.59	B B	C 0
ATOM	11364	Ň	PHE	695	77. 283 34. 366 41. 419 1. 00 22. 83	В	N N
ATOM	11365	CA	PHE	695	77. 299 35. 316 42. 531 1. 00 23. 74	В	Č
ATOM	11366	CB	PHE	695	77. 205 36. 772 42. 041 1. 00 20. 88	В	С
ATOM	11367	CG	PHE	695	78. 533 37. 397 41. 695 1. 00 19. 06	В	С

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ATOM	11368	CD1	PHE	695	79. 211	37. 042	40. 533	1.00 19.50	В	С
ATOM	11369		PHE	695	79. 096	38. 365	42.523	1.00 19.69	B	Č
ATOM	11370		PHE	695	80. 431	37. 647	40. 200	1.00 18.29	B	Č
ATOM	11371		PHE	695	80. 316	38. 977	42.199	1.00 18.53	B	Ċ
ATOM	11372	CZ	PHE	695	80. 982	38. 615	41.033	1.00 17.35	B	Č
ATOM	11373	Č	PHE	695	76. 146	35.052	43.483	1.00 24.37	B	C
ATOM	11374	0	PHE	695	76.090	35.636	44.566	1.00 25.67	В	0
ATOM	11375	N	LYS	696	75. 230	34. 173	43.089	1.00 24.40	В	N
ATOM	11376	CA	LYS	696	74.074	33.880	43.926	1.00 25.82	В	C
ATOM	11377	CB	LYS	696	73. 173	32. 813	43. 280	1.00 27.75	В	C
ATOM	11378	CG	LYS	696	72.076	32. 281	44.228	1.00 30.02	В	C
ATOM	11379	CD	LYS	696	70.680	32.287	43.615	1.00 31.63	В	C
ATOM	11380	CE	LYS	696	70.137	33. 705	43. 421	1.00 35.45	В	C
ATOM	11381	NZ	LYS	696	69.903	34. 438	44. 705	1.00 35.47	В	N
ATOM	11382	C	LYS	696	74. 402	33. 459	45.348	1.00 24.85	В	C
ATOM	11383	0	LYS	696	73. 583	33. 641	46. 242	1.00 24.94	В	0
ATOM	11384	N	GLN	697	75.587	32. 907	45.577	1.00 25.99	В	N
ATOM	11385	CA	GLN	697	75.920	32. 481	46. 931	1.00 27.33	В	C
ATOM	11386	CB	GLN	697	76. 355	31.010	46.941	1.00 29.90	В	C
ATOM	11387	CG	GLN	697	75. 290	30. 025	46.444	1.00 30.66	В	C
ATOM	11388	CD	GLN	697	75. 565	28. 593	46.889	1.00 30.92	В	C
ATOM	11389 11390	OE1 NE2	GLN	697	75. 381	28. 245	48.065	1.00 31.54	В	0
ATOM ATOM	11390	C	GLN	697	76.019	27. 761	45.958	1.00 26.21	В	N
ATOM	11391	0	GLN GLN	697 697	76.964	33. 322	47.662	1.00 26.04	В	C
ATOM	11392	N	VAL	698	77. 620 77. 125	32. 833 34. 580	48. 580 47. 270	1.00 28.31 1.00 23.16	В	0
ATOM	11394	CA	VAL	698	78. 085	35. 445	47. 270	1.00 23.10	B B	N C
ATOM	11395	CB	VAL	698	79. 411	35. 596	47. 156	1.00 21.23	В	C
ATOM	11396	CG1	VAL	698	80. 033	34. 238	46. 901	1.00 20.03	В	Č
ATOM	11397	CG2	VAL	698	79. 161	36. 335	45. 853	1.00 18.36	В	Č
ATOM	11398	C	VAL	698	77. 496	36. 829	48. 118	1.00 21.50	В	Č
ATOM	11399	ŏ	VAL	698	76. 571	37. 207	47. 404	1.00 23.06	В	0
ATOM	11400	Ň	GLU	699	78.018	37. 579	49.078	1.00 21.31	В	N
ATOM	11401	CA	GLU	699	77. 563	38. 945	49. 290	1.00 21.42	В	Č
ATOM	11402	CB	GLU	699	77. 465	39. 246	50. 785	1.00 22.73	В	č
ATOM	11403	CG	GLU	699	76. 396	38. 403	51.461	1.00 26.07	В	Č
ATOM	11404	CD	GLU	699	76.547	38. 346	52.961	1.00 29.09	B	č
ATOM	11405	0E1	GLU	699	76.343	39. 387	53.624	1.00 31.29	B	ŏ
ATOM	11406	0E2	GLU	699	76.876	37. 254	53.476	1.00 31.07	B	ŏ
ATOM	11407	C	GLU	699	78.610	39.810	48.593	1.00 21.23	B	Č
ATOM	11408	0	GLÜ	699	79.802	39. 751	48.905	1.00 21.45	B	0
ATOM	11409	N	TYR	700	78.148	40.594	47.630	1.00 19.47	B	N
ATOM	11410	CA	TYR	700	79.012	41.428	46.818	1.00 18.26	В	C
ATOM	11411	CB	TYR	700	78.830	41.001	45.368	1.00 18.24	В	C
ATOM	11412	CG	TYR	700	79.678	41.685	44.330	1.00 18.56	B	Č
ATOM	11413	CD1	TYR	700	81.071	41.698	44.422	1.00 17.75	В	C
ATOM	11414	CE1		700	81.856	42.206	43. 378	1.00 17.99	В	C
ATOM	11415	CD2		700	79.088	42. 209	43. 181	1.00 19.07	В	С
ATOM	11416	CE2	TYR	700	79. 852	42.715	42. 143	1.00 19.54	В	C

				FIG 4-234	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11417 11418 11419 11420 11421 11422 11423 11424 11425 11426 11427	CZ TYR OH TYR C TYR O TYR N LEU CA LEU CB LEU CG LEU CD1 LEU CD2 LEU C LEU	700 700 700 700 701 701 701 701 701 701	FIG. 4 - 234 81. 231	(Continued) C 0 C 0 N C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11428 11429 11430 11431 11432 11433 11434 11435 11436 11437 11438	O LEU N LEU CA LEU CB LEU CG LEU CD1 LEU CD2 LEU C LEU O LEU N ILE CA ILE	701 702 702 702 702 702 702 702 702 703 703	81. 714	O N C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11439 11440 11441 11442 11443 11444 11445 11446 11447 11448	CB ILE CG2 ILE CG1 ILE CD1 ILE C ILE O ILE N HIS CA HIS CB HIS CG HIS	703 703 703 703 703 703 704 704 704 704	82. 543 50. 967 45. 578 1. 00 13. 87 B 82. 693 52. 491 45. 775 1. 00 15. 37 B 81. 869 50. 308 46. 782 1. 00 12. 11 B 82. 714 50. 328 48. 047 1. 00 7. 95 B 82. 495 51. 251 43. 101 1. 00 15. 43 B 83. 379 50. 600 42. 548 1. 00 17. 12 B 82. 175 52. 484 42. 714 1. 00 14. 44 B 82. 866 53. 098 41. 579 1. 00 14. 11 B 82. 483 52. 356 40. 288 1. 00 12. 85 B 83. 539 52. 386 39. 224 1. 00 13. 44 B	C C C C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11449 11450 11451 11452 11453 11454 11455 11456 11457 11458	CD2 HIS ND1 HIS CE1 HIS NE2 HIS C HIS O HIS N GLY CA GLY C GLY O GLY	704 704 704 704 704 705 705 705 705	84. 363 53. 377 38. 806 1. 00 12. 54 B 83. 827 51. 293 38. 435 1. 00 12. 00 B 84. 782 51. 607 37. 578 1. 00 10. 09 B 85. 125 52. 865 37. 782 1. 00 12. 68 B 82. 533 54. 584 41. 457 1. 00 13. 37 B 81. 420 55. 007 41. 770 1. 00 15. 67 B 83. 513 55. 372 41. 027 1. 00 10. 99 B 83. 308 56. 798 40. 860 1. 00 10. 39 B 82. 807 57. 082 39. 457 1. 00 10. 13 B 83. 326 56. 536 38. 483 1. 00 11. 85 B	C N C O N C O C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11459 11460 11461 11462 11463 11464 11465	N THR CA THR CB THR OG1 THR CG2 THR C THR O THR	706 706 706 706 706 706 706	81. 805 57. 942 39. 347 1. 00 10. 36 B 81. 215 58. 272 38. 054 1. 00 9. 96 B 79. 935 59. 072 38. 232 1. 00 6. 56 B 80. 251 60. 367 38. 739 1. 00 8. 64 B 79. 025 58. 372 39. 215 1. 00 8. 26 B 82. 145 59. 052 37. 147 1. 00 11. 88 B 81. 994 59. 018 35. 927 1. 00 13. 83 B	N C C O C C

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(Continued) FIG. 4-235 37.739 ATOM 11466 707 83.114 59.741 1.00 13.21 N N ALA 36.969 C 84.075 1.00 14.57 ATOM 11467 707 60.522 В CA ALA C 11468 84.277 61.881 37.626 1.00 17.64 ATOM CB ALA 707 B 11469 85.427 59.823 36.802 1.00 13.77 C C ATOM ALA 707 В 86.445 60.484 36.639 11470 707 1.00 14.15 0 ATOM 0 ALA 36.839 ATOM 11471 N **ASP** 708 85.435 58.494 1.00 13.35 В N 86.667 57.721 36.685 ATOM 11472 CA ASP 708 1.00 12.65 В C 56. 285 55. 536 86.439 37.188 1.00 12.24 ATOM 11473 CB **ASP** 708 В 87.737 ATOM 37.453 1.00 10.05 В 11474 CG ASP 708 ATOM 11475 OD1 ASP 708 88.738 55.775 36.749 1.00 11.19 В 0 ATOM 11476 OD2 ASP 87.751 54.686 38.362 1.00 9.31 В 708 0 87.091 11477 57.696 35.202 В ATOM C ASP 708 1.00 13.18 ATOM 57.023 11478 ASP 708 86.475 34.368 1.00 13.78 В 0 0 ATOM 11479 ASP 88.156 58.423 34.891 709 1.00 12.80 В N N 58.520 ATOM 11480 ASP 709 88.679 33.534 1.00 12.65 C CA В 11481 ASP 59.825 Ċ **ATOM** 89.442 33.397 CB 709 1.00 11.74 В 90.612 **ATOM** 11482 CG **ASP** 59.912 34.366 C 709 1.00 9.63 B **ATOM** 11483 OD1 ASP 91.704 59.385 34.058 2.39 709 1.00 В 0 **ATOM** 11484 OD2 ASP 90.419 60.499 35.451 0 709 1.00 11.84 В 89.605 11485 ASP 57.366 33.167 ATOM C 709 1.00 14.57 C **ATOM** 11486 **ASP** 89.896 0 709 57.136 31.987 1.00 16.47 В 0 ATOM 11487 ASN 90.076 N 710 56.652 34.182 1.00 13.58 В N **ATOM** 11488 ASN 90.981 55.524 33.990 1.00 13.56 CA 710 В C ASN ATOM 11489 91.841 55.385 C CB 710 35.243 1.00 13.26 В ATOM 11490 CG ASN 92.987 54.440 35.059 1.00 12.07 C 710 В ATOM 11491 93.951 OD1 ASN 54.478 35.821 1.00 16.69 710 В 0 11492 ND2 ASN 92.898 53.578 ATOM 710 34.058 1.00 8.28 В N 11493 ATOM ASN 710 90.177 54.236 33.724 1.00 14.26 В C ATOM 11494 0 ASN 710 90.142 53.737 32.598 1.00 14.29 В 0 89.560 ATOM 11495 N VAL 711 53.692 34.773 1.00 13.24 В N 88. 715 52.511 ATOM 11496 CA VAL 34.652 711 1.00 12.56 В C ATOM 11497 88.835 CB VAL 51.585 35.868 1.00 11.72 C 711 В ATOM 11498 CG1 VAL 88.048 50.311 35.624 1.00 7.36 711 В $^{\rm C}_{\rm C}$ 11499 ATOM CG2 VAL 90.287 51.274 36.141 711 1.00 13.94 В ATOM 11500 C VAL 87.315 711 53.119 34.645 1.00 14.01 В C ATOM 0 11501 VAL 86.768 53.471 711 35.694 1.00 13.52 В 0 ATOM 11502 N HIS 86.746 53.249 712 33, 456 1.00 13.66 B N ATOM 11503 53.869 CA HIS 712 85.440 33.290 1.00 13.44 B C ATOM 11504 CB HIS 712 85.132 53.956 31.794 1.00 12.94 C В ATOM 11505 86.219 CG HIS 712 54.613 31.001 1.00 14.38 C В 11506 ATOM CD2 HIS 712 87. 137 55.549 31.352 1.00 15.50 В C ATOM 11507 ND1 HIS 712 86.477 54. 299 29.684 1.00 15.76 В N ATOM 11508 CE1 HIS 712 87.510 55.009 29.258 1.00 17.42 В C 87. 928 84. 293 ATOM 11509 NE2 HIS 712 55.775 30.251 1.00 16.57 В N **ATOM** HIS 11510 C 712 53.205 34.048 1.00 13.09 В C ATOM 11511 0 HIS 712 84.208 51.983 34.148 1.00 13.25 ATOM 11512 N PHE 713 83.420 54.041 1.00 13.27 34.594 В N **ATOM** 11513 CA PHE 713 82. 253 53.586 35.335 1.00 15.36 C В

> 54.759 **SUBSTITUTE SHEET (RULE 26)**

35.530

1.00 15.17

81.288

ATOM 11514 CB

PHE

713

				FIG. 4	- 236			(Continued)
ATOM 115 ATO	15 CG 16 CD1 17 CD2 18 CE1 19 CE2 20 CZ 21 C C 22 O N CA 25 CB 26 CG 27 CD NE2 30 C CD 31 O NE2 31 O NE2 33 CA 34 CB 35 CG 36 CD OE1 38 CC 36 CD OE1 37 CA 38 CC 38	ALA GLN GLN GLN	713 713 713 713 713 713 713 714 714 714 714 715 715 715 716 716 716 716 717 717 717 717 717 717	F I G. 4 80. 156 54. 464 80. 346 54. 506 78. 901 54. 11 79. 304 54. 204 77. 848 53. 803 78. 051 53. 844 81. 586 52. 48 81. 015 51. 52 81. 673 52. 644 81. 121 51. 699 81. 753 51. 923 81. 699 50. 70 82. 661 50. 81 83. 821 51. 16 82. 183 50. 49 81. 372 50. 25 80. 512 49. 38 82. 554 49. 99 82. 900 48. 64 84. 395 48. 58 85. 270 49. 08 86. 507 48. 24 86. 470 47. 02 87. 601 48. 88 82. 031 48. 13 81. 616 46. 96 81. 742 49. 00 80. 893 48. 60 81. 057 49. 54 82. 278 49. 29 79. 432 48. 57 78. 682 47. 69 79. 026 49. 51 77. 639 49. 53 77. 400 50. 70 77. 304 48. 21 76. 212 47. 69 78. 252 47. 68 78. 052 46. 41 79. 137 46. 22 79. 074 47. 23	4 36. 461 37. 841 38. 710 38. 710 38. 204 38. 204 38. 204 38. 204 39. 38. 204 30. 857 30. 857 31. 28. 770 32. 228 30. 857 32. 650 32. 487 33. 192 33. 192 33. 593 33. 593 34. 746 35. 767 32. 674 34. 746 35. 714 26. 35. 714 27. 35. 714 28. 770 39. 32. 674 31. 746 32. 746 33. 746 34. 746 35. 714 36. 829 36. 829 37. 38. 700 38.	1.00 16.29	B B B B B B B B B B B B B B B B B B B	CCCCCCONCCCONCONCCCCONCCONCCCONCCCONCCCONCCCC
ATOM 11:	553 CA 554 CB 555 CG 556 CD 557 OE1	GLN	718	78. 052 46. 41 79. 137 46. 22	7 32. 928 4 31. 858 2 30. 722 0 29. 691 9 30. 012 8 28. 449 5 33. 908 8 33. 695 0 34. 981 6 35. 953	1.00 10.32 1.00 8.83	B B	C C

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							(Continued)
					FIG. 4-238		, = 2
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11613 11614 11615 11616 11617 11618 11620 11621 11622 11623 11624 11625 11626 11627 11628 11630 11631 11632 11633 11634 11635 11637 11638 11637 11640 11641 11642 11643	CB CG1 CG2 C O N CA CB CG1 CG2 C O N CA CB CG1 CC2 C O N CA CB CCD1 CC2 C CC1 CC2 C CC1 CC2 C CC1 CC2 C C C C	VAL VAL VAL VAL VAL VAL VAL VAL VAL VASSP PHE PHE PHE PHE PHE PHE PHE	726 726 726 726 726 727 727 727 727 727	70. 409 36. 726 36. 329 1. 00 71. 727 35. 920 36. 392 1. 00 72. 246 35. 672 34. 994 1. 00 72. 763 36. 660 37. 238 1. 00 69. 789 36. 741 37. 723 1. 00 69. 858 35. 756 38. 463 1. 00 69. 198 37. 875 38. 081 1. 00 68. 548 38. 012 39. 370 1. 00 69. 387 37. 856 40. 626 1. 00 68. 961 37. 182 41. 559 1. 00 70. 568 38. 462 40. 675 1. 00 71. 389 38. 357 41. 876 1. 00 72. 859 37. 972 41. 574 1. 00 73. 693 38. 145 42. 829 1. 00 71. 396 39. 687 42. 603 1. 00 71. 738 40. 714 42. 025 1. 00 71. 738 40. 714 42. 025 1. 00 70. 998 40. 896 44. 646 1. 00 70. 146 40. 731 45. 903	10. 39 B 17. 87 B 19. 72 B	(Continued) C C C C C C C C C C C C C C C C C C
ATOM	11647	C	PHE	730	74.112 44.242 46.114 1.00 73.094 44.928 46.014 1.00 75.230 44.673 46.689 1.00		
MOTA MOTA MOTA	11651 11652 11653	CB CG CD	GLN GLN GLN	731 731 731	76. 089 45. 961 48. 569 1. 00 75. 547 44. 948 49. 536 1. 00 74. 087 45. 183 49. 854 1. 00	18. 02 B 25. 59 B 29. 48 B	C C C
ATOM ATOM ATOM	11654 11655 11656 11657	NE2 C O	GLN GLN GLN GLN	731 731 731 731	73. 263 44. 157 49. 647 1. 00 76. 124 46. 889 46. 272 1. 00 77. 060 46. 417 45. 623 1. 00	31. 32 B 32. 13 B 16. 69 B 13. 71 B	0 N C 0
ATOM ATOM ATOM ATOM	11658 11659 11660 11661	N CA CB C	ALA ALA ALA ALA	732 732 732 732	76. 425 49. 084 45. 284 1. 00 75. 718 49. 147 43. 946 1. 00	15. 59 B 15. 79 B 15. 47 B 17. 21 B	N C C C

					F I C	2 <i>A</i> -	239			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11662 11663 11664 11665 11666 11667 11668 11670 11671 11672 11673 11674 11675 11676 11677 11680 11681 11682 11683 11684 11688 11688 11688 11689 11691 11692 11693 11694 11695 11696 11701 11702 11703 11704 11705 11706	N CA CB CG SD CE CO N CA CB CG CD1 CZ2 CZ3 CH2 C O N CA CB CG CD1 CCD2 CZ CZ CC	MET	732 733 733 733 733 733 734 734 734 734 735 735 735 735 735 735 735 735 736 736 737 737 737	F I C 75. 769 77. 528 77. 737 78. 500 78. 775 77. 278 76. 781 78. 539 79. 604 78. 007 78. 673 77. 685 76. 691 75. 299 74. 785 74. 437 76. 953 75. 817 73. 449 73. 115 72. 629 79. 111 78. 491 80. 598 81. 990 81. 964 81. 321 82. 336 82. 198 81. 687 81. 511 80. 595 81. 391 79. 669 79. 517 78. 395 77. 163 78. 256 80. 789 81. 357 81. 230 82. 407 82. 151	61.673 63.571 62.278 62.730 62.457	2 3 9 46. 734 45. 382 47. 136 47. 661 47. 988 44. 719 44. 318 44. 220 42. 353 42. 650 42. 939 42. 701 42. 468 43. 376 43. 319 43. 319 43. 331 44. 788 43. 346 43. 926 44. 575 45. 920 47. 045 48. 272 46. 052 47. 270 48. 372 49. 563 41. 503 41. 882 42. 875 40. 640 40. 322 40. 684	1. 00 17. 93 1. 00 17. 27 1. 00 17. 39 1. 00 18. 98 1. 00 18. 20 1. 00 21. 42 1. 00 19. 12 1. 00 17. 30 1. 00 16. 37 1. 00 15. 48 1. 00 14. 82 1. 00 14. 06 1. 00 12. 49 1. 00 12. 15 1. 00 12. 61 1. 00 12. 61 1. 00 13. 60 1. 00 11. 75 1. 00 13. 39 1. 00 13. 13 1. 00 13. 13 1. 00 13. 13 1. 00 13. 13 1. 00 12. 17 1. 00 10. 18 1. 00 11. 23 1. 00 11. 72 1. 00 10. 18 1. 00 11. 72 1. 00 11. 30 1. 01 11. 75 1. 00 12. 02 1. 00 13. 79 1. 00 14. 20 1. 00 15. 66 1. 00 14. 01 1. 00 13. 01 1. 00 13. 01 1. 00 13. 01 1. 00 13. 01 1. 00 13. 01 1. 00 13. 01 1. 00 13. 01 1. 00 13. 01 1. 00 15. 66 1. 00 14. 01 1. 00 15. 66 1. 00 15. 66 1. 00 15. 22 1. 00 15. 22 1. 00 15. 22 1. 00 15. 22 1. 00 15. 24	B B B B B B B B B B B B B B B B B B B	(Continued) ONCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
ATOM ATOM ATOM ATOM	11707 11708 11709 11710		ASP ASP	737 737 737 737	81. 101 80. 697 80. 680 83. 737	65. 380 64. 753 66. 525 62. 811	39. 785 38. 779 40. 078 40. 912	1.00 17.61 1.00 16.59 1.00 19.23 1.00 15.17	B B B	C O O C

				FIG. 4-240	(Constituent)				
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11711 11712 11713 11714 11715 11716 11717 11718 11719 11720 11721 11722 11723 11724 11725 11726 11727 11728 11729 11730 11731 11732 11733 11734 11735 11736 11737 11738	O ASP N GLU CA GLU CB GLU CG GLU OE1 GLU OE2 GLU O GLU N ASP CA ASP CB ASP OD1 ASP OD2 ASP OD2 ASP OD ASP N HIS CA HIS CB HIS CB HIS CC HIS CC HIS O HIS CC HIS O HIS	737 738 738 738 738 738 738 739 739 739 739 739 740 740 740 740 740 740 740	84. 716 63. 560 40. 882 1. 00 14. 33 B 83. 790 61. 603 41. 453 1. 00 14. 73 B 85. 054 61. 112 41. 986 1. 00 14. 51 B 84. 829 60. 208 43. 206 1. 00 15. 23 B 84. 353 60. 935 44. 448 1. 00 16. 91 B 85. 355 61. 958 44. 956 1. 00 19. 92 B 86. 513 61. 580 45. 222 1. 00 19. 93 B 84. 985 63. 142 45. 100 1. 00 19. 97 B 85. 718 60. 319 40. 867 1. 00 13. 36 B 85. 037 59. 763 40. 005 1. 00 13. 24 B 87. 716 59. 522 39. 824 1. 00 12. 47 B 88. 809 60. 369 39. 166 1. 00 12. 46 B 89. 952 60. 717 40. 101 1. 00 16. 27 B 90. 706 61. 653 39. 751 1. 00 16. 75 B 88. 248 58. 187 40. 351 1. 00 12. 45 B 89. 735 <	N C N C				
	11738 11739 11740 11741		740 741 741 741	90. 302 55. 133 42.041 1.00 16.10 B 90. 775 57. 320 41.986 1.00 14.45 B 91. 345 57. 271 43.311 1.00 13.32 B 90. 381 57. 572 44.431 1.00 14.78 B	O N C C				
ATOM ATOM ATOM ATOM ATOM	11742 11743 11744 11745 11746	O GLY N ILE CA ILE CB ILE CG2 ILE	741 742 742 742 742	90. 763 57. 445 45. 590 1. 00 16. 71 B 89. 144 57. 946 44. 103 1. 00 14. 08 B 88. 146 58. 298 45. 111 1. 00 14. 39 B 87. 309 57. 082 45. 520 1. 00 14. 12 B 86. 121 57. 539 46. 345 1. 00 13. 12 B 86. 830 56. 336 44. 273 1. 00 13. 94 B	N C C C				
ATOM ATOM ATOM ATOM ATOM	11747 11748 11749 11750 11751	CG1 ILE CD1 ILE C ILE O ILE N ALA	742 742 742 742 743	85. 833 55. 214 44. 553 1. 00 10. 86 B 88. 892 58. 827 46. 335 1. 00 15. 89 B 88. 706 58. 350 47. 453 1. 00 17. 67 B 89. 737 59. 828 46. 108 1. 00 16. 48 B	C C O N				
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11752 11753 11754 11755 11756 11757 11758 11759	CA ALA CB ALA C ALA O ALA N SER CA SER CB SER OG SER	743 743 743 743 744 744 744 744	90. 570 60. 381 47. 157 1. 00 15. 34 B 91. 985 60. 508 46. 651 1. 00 16. 86 B 90. 149 61. 689 47. 779 1. 00 16. 53 B 90. 809 62. 153 48. 711 1. 00 18. 69 B 89. 088 62. 312 47. 287 1. 00 14. 28 B 88. 681 63. 556 47. 908 1. 00 14. 62 B 87. 369 64. 059 47. 321 1. 00 16. 50 B 86. 314 63. 152 47. 573 1. 00 22. 09 B	C C O N C C				

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(Continued) FIG. 4-241 49.390 63. 251 1.00 15.05 C 88.515 ATOM 11760 SER 744 C 88.136 62.147 49.770 1.00 17.03 0 В **ATOM** 11761 0 SER 744 88. 822 64. 223 50.229 1.00 16.05 N 11762 В ATOM N SER 745 64.051 51.666 88.712 1.00 15.38 C 11763 В CA SER 745 ATOM 88.811 65.410 52.361 1.00 15.23 C SER В 11764 CB 745 ATOM 88. 357 65.318 53.698 1.00 20.36 0 **ATOM** 11765 0G SER 745 63.360 52.103 C 1.00 14.58 11766 87.427 В ATOM C SER 745 62.334 52.773 1.00 15.64 11767 87.467 В 0 **ATOM** 0 SER 745 86. 287 85. 009 51.728 63.925 1.00 13.39 11768 THR В N **ATOM** N 746 63.355 1.00 12.46 ATOM 11769 THR 746 52.121 В C CA ATOM 11770 THR 746 83.836 64.299 51.755 1.00 13.02 В C CB 83. 858 83. 929 64.579 50.347 1.00 12.13 В 0 11771 OG1 THR **ATOM** 746 65.59952.547 1.00 6.36 В C **ATOM** 11772 CG2 THR 746 61.982 В **ATOM** 11773 746 84.748 51.513 1.00 13.71 C THR 11774 84.382 61.045 52.215 1.00 13.77 **ATOM** THR 746 В 0 0 84.948 11775 ALA 61.852 50.211 1.00 15.70 В **ATOM** 747 N N 84.698 11776 60.575 49.556 1.00 17.75 В C ATOM ALA CA 747 C 84.918 60.698 1.00 18.85 **ATOM** 11777 **ALA** 747 48.047 В CB 11778 85.579 1.00 16.94 C ATOM C **ALA** 747 59.482 50.133 В 11779 85.136 58.344 50.314 **ALA** 1.00 17.92 0 ATOM 0 747 86.828 **ATOM** 11780 59.829 50.418 1.00 15.98 N N HIS 748 **ATOM** 11781 CA 87.772 58.873 50.987 1.00 15.53 HIS 748 C 51.194 ATOM 11782 CB HIS 89.130 59.547 1.00 14.50 C 748 В 11783 90.106 58.721 51.974 **ATOM** CG HIS 1.00 12.65 В 748 90.772 58.979 C ATOM 11784 CD2 HIS 53.124 1.00 12.46 В 748 **ATOM** 11785 90.517 57.472 51.566 ND1 HIS 748 1.00 11.91 В N 56.998 91.397 11786 CE1 HIS 52.430 1.00 12.20 ATOM 748 В C 91.569 57.893 11787 ATOM NE2 HIS 748 53.384 1.00 9.44 В N 87.259 58.310 MOTA 11788 C HIS 748 52.316 1.00 15.00 В C 11789 HIS 87.272 57.097 ATOM 0 748 52.533 1.00 14.52 В 0 86. 808 86. 283 11790 **ATOM** N GLN 749 59.196 53.200 1.00 14.63 N В 58.780 ATOM 11791 CA GLN 54.496 1.00 15.23 749 В C ATOM 11792 CB **GLN** 86.045 59.999 55.378 1.00 15.87 C 749 B ATOM 11793 60.722 Č CG GLN 749 87.314 55.740 1.00 22.62 B 61.956 ATOM 11794 87.056 Ċ CD GLN 1.00 25.83 749 56.564 B ATOM 11795 86.511 OE1 GLN 749 61.873 57.664 1.00 29.51 В 0 ATOM 11796 NE2 GLN 87.443 63.116 1.00 27.64 749 56.039 В N 84. 984 84. 749 ATOM 11797 57.999 1.00 14.70 C GLN 749 54.348 B C ATOM 57.015 11798 GLN 0 749 55.054 1.00 14.10 В 0 ATOM 11799 HIS 84.147 58.440 N 750 53.415 1.00 13.44 В N ATOM 11800 CA 82.865 57.808 53.174 HIS 750 1.00 12.63 В C 82. 021 11801 ATOM CB HIS 750 58.685 52.247 1.00 13.59 В C ATOM 11802 CG HIS 750 80.587 58. 272 52.176 1.00 12.41 B C 11803 79.475 ATOM CD2 HIS 750 58.823 52.713 1.00 13.33 В C 11804 80.175 57.128 ATOM ND1 HIS 750 51.530 1.00 12.98 В N ATOM 11805 CE1 HIS 750 78.869 56.992 51.673 1.00 14.44 B C ATOM 11806 NE2 HIS 750 78.419 58.007 52.386 1.00 13.43 N B 11807

SUBSTITUTE SHEET (RULE 26)

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ATOM

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245/246

				,							(Con	tinued)
					FIG	. 4 -	2 4 2				(COII	unueu
ATOM	11809	N	ILE	751	83. 885	56. 203	51.638	1 00	13.03	В	N	
ATOM	11810	CA	ILE	751		54. 875	51.077		12.47	В	Č	
ATOM	11811	CB	ILE	751		54. 838	49. 814		13.01	B	č	
ATOM	11812		ILE	751		55. 361	50.137		12.55	В	С	
ATOM	11813	CG1		751		53. 395	49. 287		12.09	В	С	
ATOM	11814	CD1		751		53. 240	47.939		11.16	В	C	
ATOM	11815	C	ILE	751		53. 893	52. 111		12.65	В	C	
ATOM	11816	0	ILE	751		52. 790	52. 241		12.49	В	0	
ATOM	11817	N	TYR	752		54. 284	52.858		13.74	В	N	
ATOM	11818	CA	TYR	752 752		53. 364 53. 883	53. 850 54. 379		14.04 11.26	B B	C C	
ATOM ATOM	11819 11820	CB CG	TYR TYR	752 752		53. 468	53. 472	1.00	9.86	В	C	
ATOM	11821	CD1		752		52. 132	53. 408		10.53	В	Č	
ATOM	11822		TYR	752		51.712	52. 502	1.00	9.48	B	č	
ATOM	11823		TYR	752		54. 383	52.608	1.00	9.66	B	Č	
ATOM	11824		TYR	752		53. 974	51.692	1.00	8.36	В	C	
ATOM	11825	CZ	TYR	752		52. 639	51.646	1.00	9.94	В	C	
ATOM	11826	OH	TYR	752		52. 223	50. 739		10.79	В	0	
ATOM	11827	C	TYR	752		53.067	54. 973		13.42	В	C	
MOTA	11828	0 M	TYR	752 753		51.972	55. 524 55. 295		13.56	В	0	
ATOM ATOM	11829 11830	N CA	THR THR	753 753		54. 040 53. 864	56. 330		14. 48 14. 27	B B	N C	
ATOM	11831	CB	THR	753		55. 187	56.618		13.68	В	Č	
ATOM	11832	0G1	THR	753		56. 136	57. 130		17.48	B	ŏ	
ATOM	11833		THR	753		54. 987	57.629	1.00	7.20	B	Č	
ATOM	11834	С	THR	753		52. 849	55.815	1.00	16.15	В	С	
ATOM	11835	0	THR	753		51.894	56. 508		18.93	. В	0	
ATOM	11836	N	HIS	754		53.056	54. 589		15.38	В	N	
ATOM	11837	CA	HIS	754 754		52. 163	53. 999		16.06	В	C	
ATOM ATOM	11838 11839	CB CG	HIS HIS	754 754		52. 666 52. 128	52. 620 52. 162		15. 26 16. 39	B B	C	
ATOM	11840		HIS	754 754		51.362	51.095		15. 75	В	C	
ATOM	11841		HIS	754		52. 353	52. 850		17.30	В	N	
ATOM	11842		HIS	754		51.750	52. 228		15.86	B	Ċ	
ATOM	11843		HIS	754		51.141	51.161		17.13	B	Ň	
ATOM	11844	C	HIS	754		50. 731	53.886	1.00	16.28	В	C	
ATOM	11845	0	HIS	754		49. 788	54. 238		17.31	В	0	
ATOM	11846	N	MET	755		50. 564	53. 383		15.98	В	N	
ATOM	11847	CA	MET	755		49. 234	53. 250		16.05	В	C	
ATOM	11848	CB	MET	755		49. 300	52. 573		15.41	В	C	
ATOM ATOM	11849 11850	CG SD	MET MET	755 755		49. 542 49. 308	51. 081 50. 322		17. 11 18. 41	B B	C	
ATOM	11851	CE	MET	755		50. 855	50. 742		20. 74	В	S C	
ATOM	11852	C	MET	755		48. 582	54. 623		15. 38	В	Č	
ATOM	11853	Ŏ	MET	755		47. 390	54. 783		13.30	В	ŏ	
ATOM	11854	N	SER	756		49.371	55.614		15.36	В	N	
ATOM	11855	CA	SER	756		48. 833	56.946		18.52	В	С	
ATOM	11856	CB	SER	756		49. 903	57. 878		18.88	В	C	
ATOM	11857	0G	SER	756	85. 723	50. 257	57. 477	1.00	18. 74	В	0	

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		_	000	550	00 515	40 000	57. 462	1.00 19.14	В	С
ATOM	11858	C	SER	756	82.515	48. 282	57. 975	1.00 19.14	В	Ö
ATOM	11859	0	SER	756	82.464	47. 158	57. 324	1.00 13.34	В	N
ATOM	11860	N	HIS	757	81.435	49.048	57. 770	1.00 17.00	В	Č
ATOM	11861	CA	HIS	757	80.134	48. 549	57. 770	1.00 19.20	В	Č
ATOM	11862	CB	HIS	757	78. 990	49.486	58. 095	1.00 18.83	В	Č
ATOM	11863	CG	HIS	757	78. 983	50.794	57. 666	1.00 21.13	В	Č
ATOM	11864		HIS	757 757	78. 697	52.046	59.447	1.00 22.10	В	Ň
ATOM	11865	ND1	HIS	757 757	79. 230	50.899	59. 820	1.00 22.02	В	Č
ATOM	11866		HIS	757 757	79.096	52. 159	58. 758	1.00 24.81	В	N
ATOM	11867		HIS	757 757	78. 772	52.876	57. 120	1.00 24.81	В	C
ATOM	11868	Ç	HIS	757 757	79.866	47. 190 46. 251	57. 772	1.00 16.54	В	Ö
ATOM	11869	0	HIS	757 750	79.416	40. 251	55. 828	1.00 17.93	В	N
ATOM	11870	N	PHE	758 758	80. 158	47. 103	55. 052	1.00 11.35	В	Ċ
ATOM	11871	CA	PHE	758 758	79. 926 80. 286	46. 138	53. 586	1.00 15.70	B	Č
ATOM	11872	CB	PHE	758 758	79. 952	40. 136	52. 677	1.00 10.77	В	Č
ATOM	11873	CG	PHE	758 758	79. 952	44. 790	52. 251	1.00 10.11	В	Č
ATOM	11874		PHE	758 758	80. 941	44. 120	52. 254	1.00 6.53	В	č
ATOM	11875		PHE PHE	758	78. 334	43.716	51.409	1.00 9.32	В	č
ATOM	11876	CE1	PHE	758	80. 638	43. 045	51.403	1.00 6.01	В	Č
ATOM	11877 11878	CE2 CZ	PHE	758	79. 340	42. 836	50. 991	1.00 2.78	В	Č
ATOM ATOM	11879	C	PHE	758	80. 697	44.674	55. 560	1.00 20.68	B	Č
	11880	0	PHE	758	80. 110	43. 631	55.851	1.00 21.00	B	ŏ
ATOM ATOM	11881	N	ILE	759	82.014	44.811	55.654	1.00 23.57	В	Ň
ATOM	11882	CA	ILE	759	82. 858	43. 722	56.117	1.00 25.05	B	Ċ
ATOM	11883	CB	ILE	759	84. 364	44. 129	56.069	1.00 25.44	В	Č
ATOM	11884	CG2		759	84. 994	44. 041	57. 437	1.00 28.98	B	Č
ATOM	11885	CG1	ILE	759		: 43. 189	55. 142	1.00 26.52	B	Č
ATOM	11886	CDI	ILE	759	84. 706	43. 263	53. 704	1.00 26.84	B	Č
ATOM	11887	C	ILE	759	82. 441	43. 318	57. 529	1.00 25.34	B	Č
ATOM	11888	ŏ	ILE	759	82. 420	42. 136	57. 866	1.00 25.50	B	Õ
ATOM	11889	Ň	LYS	760	82. 081	44. 299	58.346	1.00 26.11	В	N
ATOM	11890	CA	LYS	760	81.671	44.012	59. 713	1.00 26.62	В	C
ATOM	11891	CB	LYS	760	81.444	45. 300	60.487	1.00 26.43	В	C
ATOM	11892	CG	LYS	760	82.178	45. 298	61.792	1.00 29.00	В	C
ATOM	11893	CD	LYS	760	83.666	45. 271	61.537	1.00 28.96	В	C
ATOM	11894	CE	LYS	760	84.139	46.665	61.250	1.00 30.01	В	C.
ATOM	11895	NZ	LYS	760	83.776	47.523	62.420	1.00 31.29	В	N
ATOM	11896	C	LYS	760	80.406	43.179	59.740	1.00 27.08	В	C
ATOM	11897	Ō	LYS	760	80.312	42.200	60.473	1.00 28.46	В	0
ATOM	11898	N	GLN	761	79.431	43. 581	58.940	1.00 28.08	В	N
ATOM	11899	CA	GLN	761	78.170	42.866	58.844	1.00 29.69	В	C
ATOM	11900	CB	GLN	761	77. 213	43.652	57. 942	1.00 31.26	В	C
ATOM	11901	CG	GLN	761	76.072	42.855	57. 347	1.00 34.99	В	C
ATOM	11902	CD	GLN	761	76.477	42.140	56.072	1.00 37.85	В	C
ATOM	11903	0E1		761	76.800	42.775	55.062	1.00 37.29	В	0
ATOM	11904	NE2		761	76.464	40. 808	56.112	1.00 39.80	В	N
ATOM	11905	C	GLN	761	78. 401	41.456	58. 295	1.00 30.00	В	C
ATOM	11906	0	GLN	761	77. 791	40. 494	58. 753	1.00 31.14	В	0
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						(Continued)
					FIG. 4-245	(Continued)
ATOM	11956	04	NAG	901	24. 256 39. 836 11. 036 1. 00 49. 01 E	0
ATOM	11957	C5	NAG	901	23. 545 39. 104 13. 219 1. 00 49. 11 E	C
ATOM	11958	05	NAG	901	23. 858 38. 173 14. 276 1. 00 47. 99 E	0
ATOM	11959	C6	NAG	901	22. 143 38. 804 12. 731 1. 00 50. 99 E	C
ATOM	11960	06	NAG	901	21. 706 39. 781 11. 793 1. 00 53. 28 E 34. 526 67. 450 4. 248 1. 00 29. 71 E	0 C
ATOM	11961	C1	NAG	902		Č
ATOM	11962	C2	NAG	902		N N
ATOM	11963	N2 C7	NAG NAG	$\frac{902}{902}$	34. 077 65. 638 2. 692 1. 00 35. 02 E 33. 181 64. 660 2. 610 1. 00 35. 78 E	Č
ATOM ATOM	11964 11965	07	NAG	902	32. 213 64. 701 1. 852 1. 00 37. 59 E	ŏ
ATOM	11966	C8	NAG	902	33. 392 63. 449 3. 503 1. 00 37. 18 E	Č
ATOM	11967	C3	NAG	902	33. 927 67. 915 1. 848 1. 00 31. 67 E	Č
ATOM	11968	03	NAG	902	33. 032 67. 583 0. 794 1. 00 34. 76 E	0
ATOM	11969	C4	NAG	902	33.753 69.386 2.248 1.00 31.76 E	C
ATOM	11970	04	NAG	902	34. 037 70. 238 1. 144 1. 00 30. 03 E	0
ATOM	11971	C5	NAG	902	34.701 69.674 3.412 1.00 30.64 E	C
ATOM	11972	05	NAG	902	34. 332 68. 844 4. 526 1. 00 30. 02 E	0
ATOM	11973	C6	NAG	902	34.720 71.114 3.892 1.00 30.81 E	C
ATOM	11974	06	NAG	902	33.457 71.512 4.409 1.00 34.26 E	0
ATOM	11975	CI	NAG	903	64. 239 77. 734 14. 341 1. 00 27. 20 E	C
ATOM	11976	C2	NAG	903	63. 984 78. 203 12. 917 1. 00 26. 96 E	C
ATOM	11977	N2	NAG	903	63. 551 77. 080 12. 116 1. 00 25. 19 E	
ATOM	11978	C7	NAG	903	62. 349 77. 076 11. 551 1. 00 24. 99 E	
ATOM	11979	07	NAG	903	62.121 76.492 10.490 1.00 25.88 E 61.222 77.800 12.272 1.00 23.55 E	
ATOM	11980	C8	NAG	903	61.222 77.800 12.272 1.00 23.55 E 65.253 78.817 12.325 1.00 29.00 E	
ATOM	11981 11982	C3 03	NAG NAG	903 903	64. 947 79. 400 11. 066 1. 00 29. 62 E	
ATOM ATOM	11983	C4	NAG	903	65. 814 79. 900 13. 248 1. 00 30. 83 E	
ATOM	11984	04	NAG	903	67. 092 80. 316 12. 778 1. 00 31. 15 E	
ATOM	11985	C5	NAG	903	65.929 79.389 14.690 1.00 30.71 E	
ATOM	11986	05	NAG	903	64.669 78.842 15.133 1.00 30.11 E	
ATOM	11987	C6	NAG	903	66. 276 80. 502 15. 659 1. 00 32. 26 E	
ATOM	11988	06	NAG	903	65. 937 80. 144 16. 993 1. 00 35. 52 E	
ATOM	11989	C1	NAG	904	56.857 73.229 -0.933 1.00 21.65 E	C
ATOM	11990	C2	NAG	904	58. 289 73. 099 -1. 475 1. 00 21. 59 E	
ATOM	11991	N2	NAG	904	58.532 71.758 -1.961 1.00 21.40 E	
ATOM	11992	C7	NAG	904	58. 567 71. 523 -3. 267 1. 00 20. 76 E	
ATOM	11993	07	NAG	904	58.745 72.412 -4.104 1.00 18.55 E	0
ATOM	11994	C8	NAG	904	58. 371 70. 080 -3. 709 1. 00 20. 74 E	
ATOM	11995	C3	NAG	904		
ATOM	11996	03	NAG	904	60.611 73.413 -1.009 1.00 22.81 E	
ATOM	11997	C4	NAG	904	59. 022 74. 832 0. 129 1. 00 22. 85 E	
ATOM	11998	04	NAG	904	59. 986 75. 217 1. 101 1. 00 24. 62 E	0
ATOM	11999	. C5	NAG	904	57. 634 74. 781 0. 737 1. 00 22. 86 E	
ATOM	12000	05 C6	NAG	904	56. 672 74. 506 -0. 297 1. 00 21. 95 E	
ATOM	12001	C6	NAG	904	57. 232 76. 083 1. 385 1. 00 24. 39 E 57. 196 77. 133 0. 430 1. 00 31. 81 E	
ATOM ATOM	12002 12003	06 C1	NAG NAG	904 905	57. 196 77. 133 0. 430 1. 00 31. 81 E 49. 743 85. 075 37. 084 1. 00 31. 93 E	
ATOM	12003	C2	NAG	905	49.010 86.230 37.756 1.00 33.35 E	
VI OUT	14004	Ų4	IMU	300	70. UIU 00. 200 01. 100 1. 00 00. 00 E	U

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										(Continued)
					FIG	. 4 -	2 4 6			
ATOM	12005	N2	NAG	905	47.823	86. 586	37.012	1.00 34.30	Е	N
ATOM	12006	C7	NAG	905		86.099	37.395	1.00 35.18	E	C
ATOM	12007	07	NAG	905		85.888	38. 578	1.00 36.47	Е	0
ATOM	12008	C8	NAG	905		85. 786	36. 303	1.00 37.15	E	C
ATOM	12009	C3	NAG	905		87.416	37. 924	1.00 33.45	E	C
ATOM	12010	03	NAG	905		88. 512	38. 495	1.00 33.93	E	0
ATOM	12011	C4	NAG	905		86.945	38.863	1.00 35.37	E	C
ATOM	12012	04	NAG	905		88. 009	39. 193	1.00 35.45	E	0
ATOM	12013	C5	NAG	905		85. 773	38. 215	1.00 34.39	E	C
ATOM	12014	05	NAG	905		84. 684	37.887	1.00 32.56	E	0
ATOM	12015	C6	NAG	905		85. 212	39. 214	1.00 36.29	E	C
ATOM	12016	06	NAG	905		84. 936	40.459	1.00 35.52	E E	0
ATOM	12017	C1 C2	NAG	906	128. 439	74. 792	56.371	1.00 36.45	E E	C C
ATOM ATOM	12018 12019	N2	NAG NAG	906 906	127. 977 126. 880	75. 856 75. 335	55.375 54.586	1.00 37.00 1.00 37.17	E E	N N
ATOM	12019	C7	NAG	906		75. 871	54. 690	1.00 37.17	E	C
ATOM	12020	07	NAG	906		76. 427	55. 714	1.00 38.52	E	Ö
ATOM	12021	C8	NAG	906		75. 782	53. 471	1.00 36.25	Ë	č
ATOM	12023	C3	NAG	906		76. 265	54. 465	1.00 38.66	Ē	č
ATOM	12024	03	NAG	906		77. 334	53. 625	1.00 39.59	Ē	ŏ
ATOM	12025	C4	NAG	906		76.704	55. 308	1.00 39.58	Ē	č
ATOM	12026	04	NAG	906		76.975	54.460	1.00 41.48	Ē	Õ
ATOM	12027	C5	NAG	906		75.602	56.312	1.00 40.24	E	Ċ
ATOM	12028	05	NAG	906	129. 556	75.268	57.133	1.00 38.27	E	0
ATOM	12029	C6	NAG	906		76.032	57.255	1.00 41.89	E	С
ATOM	12030	06	NAG	906	131.906	75.162	58.378	1.00 46.70	Е	0
ATOM	12031	C1	NAG	907		72. 294	25.405	1.00 33.54	E	C
ATOM	12032	C2	NAG	907		73.454	25.478	1.00 35.73	E	C
ATOM	12033	N2	NAG	907		74. 367	26. 540	1.00 37.97	E	Ŋ
ATOM	12034	C7	NAG	907		74. 400	27. 644	1.00 41.34	E	C
ATOM	12035	07	NAG	907		73. 403	28. 094	1.00 42.96	E	0
ATOM	12036	C8	NAG	907		75. 739	28. 352	1.00 42.60	E	C C
ATOM	12037	C3	NAG	907		74. 167	24. 126	1.00 36.63	E	
ATOM	12038	03	NAG	907		75. 253	24. 154	1.00 38.28	E	0
ATOM ATOM	12039 12040	C4 04	NAG NAG	907 907		73. 148 73. 758	23. 047 21. 763	1.00 35.89	E	C
ATOM	12040	C5	NAG	907		71. 995	23. 075	1.00 35.82 1.00 35.12	E	0
ATOM	12041	05	NAG	907		71.377	24. 380	1.00 33.12	E E	C
ATOM	12042	C6	NAG	907		70. 913	22.057	1.00 32.01	E	C 0
ATOM	12044	06	NAG	907		70.083	22. 478	1.00 38.44	E	0
ATOM	12045	C1	NAG	908		64. 129	12. 586	1.00 33.44	E	0 C C
ATOM	12046	C2	NAG	908		65. 101	11.602	1.00 36.51	Ë	Č
ATOM	12047	N2	NAG	908		66. 365	12. 269	1.00 40.33	Ë	N
ATOM	12048	C7	NAG	908		66.962	12. 148	1.00 43.03	Ē	Ĉ
ATOM	12049	07	NAG	908		66. 434	12.500	1.00 45.77	Ē	ŏ
ATOM	12050	C8	NAG	908		68. 349	11.529	1.00 43.86	Ē	č
ATOM	12051	C3	NAG	908		65. 325	10.380	1.00 37.11	Ē	Č
ATOM	12052	03	NAG	908		66.122	9.426	1.00 37.35	Ē	Õ
ATOM	12053	C4	NAG	908	96.945	63. 975	9.760	1.00 36.97	Е	С

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										(Continued)
					FIG	. 4 -	247			(Continued)
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ATOM	12054	04	NAG	908	96.049	64. 165	8.668	1.00 36.08	E	0
ATOM	12055	C5	NAG	908	96. 291	63. 106	10.841	1.00 35.43	E	C
ATOM	12056	05	NAG	908	97. 215	62.906	11.930	1.00 33.34	E	0
ATOM	12057	C6	NAG	908	95. 890	61.735	10.341	1.00 36.72 1.00 38.75	E E	C 0
ATOM	12058	06	NAG	908	95.085	61.057	11. 296 11. 987	1.00 55.75	E	C
ATOM	12059	Cl	NAG	909	106.501	80. 407 81. 255	11. 967	1.00 55.21	E	Č
ATOM	12060	C2	NAG	909 909	105. 627 105. 631	82.658	11. 427	1.00 55.10	E	N
ATOM ATOM	12061 12062	N2 C7	NAG NAG	909	105. 031	83. 259	11. 828	1.00 56.83	Ë	Č
ATOM	12062	07	NAG	909	107. 685	83. 526	11.066	1.00 55.16	Ē	Ö
ATOM	12064	C8	NAG	909	106.838	83.620	13. 305	1.00 56.25	E	C
ATOM	12065	C3	NAG	909	104. 195	80.724	11.087	1.00 56.36	Е	С
ATOM	12066	03	NAG	909	103.396	81.452	10.166	1.00 58.58	E	0
ATOM	12067	C4	NAG	909	104.176	79.229	10.744	1.00 56.19	Е	C
ATOM	12068	04	NAG	909	102.855	78.716	10.862	1.00 55.29	E	0
ATOM	12069	C5	NAG	909	105. 117	78. 478	11.692	1.00 56.24	E	C
ATOM	12070	05	NAG	909	106.446	79.028	11.600	1.00 56.65	E.	0
ATOM	12071	C6	NAG	909	105. 230	76. 996	11.381	1.00 57.38	E	C
ATOM	12072	06	NAG	909	106.370	76. 423	12.010	1.00 55.01	E	0
ATOM	12073	Cl	NAG	910	105. 213	38. 428	20.006	1.00 34.33 1.00 37.27	E E	C
ATOM	12074	C2 N2	NAG NAG	910 910	106. 113 107. 447	37. 293 37. 789	19. 498 19. 211	1.00 37.27	E	N N
ATOM ATOM	12075 12076	C7	NAG	910	107. 447	36. 984	19. 368	1.00 40.00	E	Č
ATOM	12070	07	NAG	910	109.013	36. 771	20. 465	1.00 42.65	Ë	ŏ .
ATOM	12078	C8	NAG	910	109.047	36. 295	18. 126	1.00 42.65	Ē	Č
ATOM	12079	C3	NAG	910	105. 504	36.650	18. 245	1.00 37.60	Ē	Č
ATOM	12080	03	NAG	910	106. 296	35. 547	17.831	1.00 38.44	E	0
ATOM	12081	C4	NAG	910	104.084	36. 182	18.551	1.00 36.63	Е	C
ATOM	12082	04	NAG	910	103. 489	35.616	17. 388	1.00 37.52	E	0
ATOM	12083	C5	NAG	910	103. 274	37. 387	19.037	1.00 35.81	E	C
ATOM	12084	05	NAG	910	103. 883	37. 930	20. 229	1.00 34.96	E	0
ATOM	12085	C6	NAG	910	101.838	37.042	19.385	1.00 34.79	E	C
ATOM	12086	06	NAG	910	101. 781	36. 089	20. 437	1.00 34.77	E	0
TER	12087	Λ	NAG	910	E9 49E	00 704	10 179	1 00 10 60	E	0
ATOM	12088	0	НОН	1	53. 435	80. 704 78. 703	18. 172 26. 320	1.00 10.60 1.00 21.03	W	0 0
ATOM ATOM	12089 12090	0 0	HOH HOH	2 3	57. 473 65. 386	56.077	37. 040	1.00 21.03	W	0
ATOM	12091	0	HOH	4	56. 235	76. 520	22. 816	1.00 14.76	Ÿ	0
ATOM	12092	ŏ	НОН	5	58. 127	60.758	28.066	1.00 4.57	Ÿ	ŏ
ATOM	12093	.ŏ	НОН	6	40. 099	59.877	48. 410	1.00 16.00	Ÿ	ŏ
ATOM	12094	Ŏ	НОН	7	29. 796	47. 323	37. 410	1.00 24.76	Ÿ	ŏ
ATOM	12095	Ŏ	НОН	8	38. 634	67. 195	51.371	1.00 22.65	Ŵ	Ō
ATOM	12096	0	HOH	9	41.732	52.103	37. 673	1.00 13.34	W	0
ATOM	12097	0	HOH	10	79. 275	54. 159	21.409	1.00 15.53	W	0
ATOM	12098	0	HOH	11	65. 287	66.160	35. 128	1.00 7.29	W	0
ATOM	12099	0	НОН	12	79. 267	49. 364	26. 780	1.00 14.00	W	0
ATOM	12100	0	HOH	13	67. 989	56. 792	26. 833	1.00 20.21	W	0
ATOM	12101	0	НОН	14.	68. 995	70. 138	19.815	1.00 12.98	W.	0
ATOM	12102	0	НОН	15	59. 193	63. 441	21. 787	1.00 5.68	W	0

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										(Continued)
					FIG.	. 4 -	2 4 8			(00_0_0
ATOM	12103	0	НОН	16	49.896	66. 700	47. 886	1.00 13.21	W	0
ATOM	12103	ő	НОН	17		53.043	50.567	1.00 20.65	W.	Ö
ATOM	12105	ŏ	НОН	18		69.817	52.424	1.00 34.74	W	0
ATOM	12106	ŏ	НОН	19		69.650	29.378	1.00 25.18	W	0
ATOM	12107	Õ	HOH	20		61.115	48. 431	1.00 18.77	W	0
ATOM	12108	Ō	НОН	21		85. 282	28.107	1.00 27.06	W	0
ATOM	12109	0	HOH	22		63. 930	21.686	1.00 29.16	W	0
ATOM	12110	0	HOH	23	43.777 8	87. 394	23. 730	1.00 9.96	W	0
ATOM	12111	0	HOH	24		67. 109	30. 405	1.00 21.66	W	0
ATOM	12112	0	HOH	25		80. 303	31.025	1.00 34.33	₩	0
ATOM	12113	0	HOH	26		66.634	22.568	1.00 10.18	W	0
ATOM	12114	0	НОН	27		54.838	52. 427	1.00 29.90	Ä	0
ATOM	12115	0	НОН	28		80.961	23. 145	1.00 17.51	W	0
ATOM	12116	0	НОН	29		71.484	27. 824	1.00 34.92	W	0
ATOM	12117	0	HOH	30		57.060	34. 794	1.00 28.05	W	0
ATOM	12118	0	HOH	31		72.092	24. 987	1.00 14.46	W	0
ATOM	12119	0	HOH	32		84. 543	25. 502	1.00 22.75 1.00 12.55	W	0
ATOM	12120	0	HOH	33		63. 840 47. 441	46. 551 47. 587	1.00 12.00	W W	0
ATOM	12121 12122	0 0	HOH HOH	34 35		56.510	44. 904	1.00 23.33	W	0
ATOM ATOM	12122	0	НОН	36		59. 222	42. 224	1.00 30.31	W	0
ATOM	12123	0	HOH	37		64. 199	47. 510	1.00 21.69	W	0
ATOM	12125	ő	НОН	38		70.385	33. 904	1.00 24.19	Ÿ	ŏ
ATOM	12126	ő	НОН	39		47.056	34. 998	1.00 24.19	W	ŏ
ATOM	12127	ŏ	HOH	40		49. 571	32. 910	1.00 22.85	W	Ŏ
ATOM	12128	Ö	НОН	41		53.516	39. 573	1.00 12.47	W	Ö
ATOM	12129	Ö	НОН	$\overline{42}$		48. 248	21.021	1.00 24.35	W	Ō
ATOM	12130	Õ	НОН	43		53.457	19.457	1.00 32.23	W	0
ATOM	12131	0	НОН	44		61.003	21.232	1.00 19.07	¥	0
ATOM	12132	0.	HOH	45	51.713	50. 325	19.619	1.00 36.05	W	0
ATOM	12133	0	HOH	46		58.001	59.062	1.00 20.53	₩	0
ATOM	12134	0	HOH	47		54.978	15. 598	1.00 20.74	¥	0
ATOM	12135	0	HOH	48		51.103	23. 882	1.00 16.65	W	0
ATOM	12136	0	HOH	49		66. 281	21.097	1.00 18.82	W	0
ATOM	12137	0	НОН	50		72. 589	-9.525	1.00 19.51	Ä	0
ATOM	12138	0	HOH	51		47. 337	39. 374	1.00 16.49	Ŋ	0
ATOM	12139	0	HOH	52		68. 673	61. 331	1.00 26.41	W	0
ATOM	12140	0	HOH	53		48. 947	47. 621	1.00 17.49	W	0
ATOM	12141	0	HOH	54		82. 021	10.956	1.00 24.56	W	0
ATOM	12142	0	HOH	55 56		45. 427	40.043	1.00 35.52	W	0
ATOM	12143	0	HOH	56		60.491	43. 209	1.00 10.79	W	0
ATOM	12144	0	HOH HOH	57 58		62. 843 55. 643	34. 752 2. 123	1.00 17.19 1.00 19.51	M. M.	0
ATOM ATOM	12145 12146	0	нон НОН	56 59		45. 985	50.017	1.00 19.51	H H	0
ATOM	12140	0	НОН	60		40. 965 70. 566	0.317	1.00 22.18	n W	0
ATOM	12148	0	HOH	61		69. 597	25. 094	1.00 32.17	MA.	0
ATOM	12149	0	НОН	62		79. 521	14. 538	1.00 13.27	TV	0
ATOM	12150	ŏ	НОН	63		86. 907	16. 122	1.00 21.54	W,	0
ATOM	12151	ŏ	НОН	64		54. 337	14. 938	1.00 22.27	Ÿ	ŏ
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						(Continued)
					FIG. 4-249	(Continued)
ATOM	12152	0	НОН	65	37.711 84.458 31.782 1.00 38.65 W	0
ATOM	12153		НОН	66	41.832 62.441 48.190 1.00 23.50 W	0
ATOM	12154		HOH	67	56. 514 63. 214 39. 402 1. 00 20. 39 W	0
ATOM	12155		НОН	68	48. 166 60. 456 42. 122 1. 00 37. 55 W	0
ATOM ATOM	12156 12157		HOH HOH	69 70	52.076 51.584 45.757 1.00 22.02 W 47.607 61.634 15.612 1.00 34.50 W	0
ATOM	12158		HOH	71	47.607 61.634 15.612 1.00 34.50 W 39.108 76.636 34.882 1.00 24.21 W	0 0
ATOM	12159		НОН	72	62. 894 85. 163 44. 724 1. 00 38. 05 W	0
ATOM	12160	Ŏ	НОН	73	49. 937 51. 963 48. 658 1. 00 25. 50 W	ŏ
ATOM	12161	0	HOH	74	32.972 63.405 9.645 1.00 31.16 W	Ö
ATOM	12162	0	HOH	75	76.481 50.940 55.523 1.00 8.02 W	0
ATOM	12163	0	НОН	76	54. 751 68. 666 -3. 038 1. 00 19. 33 W	0
ATOM	12164	0	HOH	77	69. 797 76. 851 37. 550 1. 00 38. 44 W	0
ATOM ATOM	12165 12166	0	НОН НОН	78 70	60.195 69.793 56.043 1.00 27.75 W	0
ATOM	12167	0	ноп НОН	79 80	68. 721 77. 775 28. 423 1. 00 14. 61 W 76. 538 41. 044 29. 727 1. 00 24. 17 W	0 0
ATOM	12168	0	НОН	81	27. 643 63. 804 39. 245 1. 00 20. 70 W	0
ATOM	12169	ŏ	НОН	82	42.573 57.621 42.066 1.00 19.56 W	0
ATOM	12170	0	HOH	83	51. 219 56. 139 24. 829 1. 00 41. 31 W	Ŏ
ATOM	12171	0	HOH	84	64. 281 54. 295 25. 797 1. 00 15. 83 W	Ō
ATOM	12172	0	НОН	85	48. 093 54. 052 46. 307 1. 00 38. 41 W	0
ATOM	12173	0	HOH	86	37.006 52.225 21.202 1.00 23.83 W	0
ATOM ATOM	12174 12175	0	НОН	87	44. 149 74. 948 5. 314 1. 00 17. 55 W	0
ATOM	12176	0	HOH HOH	88 89	72.912 75.091 28.633 1.00 25.98 \\ 52.329 67.860 33.481 1.00 8.31 \\	0
ATOM	12177	0	НОН	90	52. 329 67. 860 33. 481 1. 00 8. 31 W 66. 266 74. 773 42. 238 1. 00 16. 00 W	0 0
ATOM	12178	ŏ	HOH	91	59. 283 77. 076 9. 072 1. 00 41. 29 W	0
ATOM	12179	0	НОН	92	77. 526 46. 454 20. 254 1. 00 34. 51	Ö
ATOM	12180	0	HOH	93	59.751 56.673 29.191 1.00 24.40 W	Ö
ATOM	12181	0	НОН	94	43. 531 63. 248 14. 122 1. 00 22. 64 W	0
ATOM	12182	0	НОН	95	56. 677 73. 257 -8. 550 1. 00 18. 65 W	0
ATOM ATOM	12183 12184	0	НОН	96	64. 366 82. 016 33. 202 1. 00 24. 81 W	0
ATOM	12185	0	H0H H0H	97 98	58. 839 62. 776 26. 537 1. 00 11. 00 W 52. 478 72. 152 3. 092 1. 00 13. 58 W	0
ATOM	12186	Ö	НОН	99	52.478 72.152 3.092 1.00 13.58 W 59.860 59.389 29.429 1.00 20.06 W	0
ATOM	12187	Ö	НОН	100	64. 047 73. 184 44. 557 1. 00 15. 66 W	0
ATOM	12188	0	НОН	101	44. 369 74. 978 38. 087 1. 00 11. 11 W	ŏ
ATOM	12189	0	HOH	102	61.861 50.833 14.510 1.00 31.09 W	Ö
ATOM	12190	0	HOH	103	40.708 73.940 22.137 1.00 13.81 W	0
ATOM	12191	0	HOH	104	51. 853 81. 601 16. 339 1. 00 16. 73 W	0
ATOM	12192	0	HOH	105	59. 699 55. 348 63. 144 1. 00 20. 67 W	0
ATOM ATOM	12193 12194	0 0	HOH HOH	106 107	45.186 81.560 8.416 1.00 13.89 W 37.516 59.183 48.946 1.00 20.72 W	0
ATOM	12195	0	нон НОН	107	**	0
ATOM	12196	Ö	НОН	109	22. 032 56. 444 27. 934 1. 00 30. 26 W 65. 773 63. 945 59. 504 1. 00 15. 82 W	· 0
ATOM	12197	Ŏ	НОН	110	45. 931 73. 798 1. 832 1. 00 25. 56	0
ATOM	12198	0	HOH	111	29. 602 40. 898 24. 033 1. 00 25. 93 W	0
ATOM	12199	0	НОН	112	19.080 57.313 26.663 1.00 20.07 W	Ŏ
ATOM	12200	0	HOH	113	61. 355 50. 296 11. 653 1. 00 20. 49 W	0
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						(Continued)
					FIG. 4-250	(00111111111111111111111111111111111111
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	12201 12202 12203 12204 12205 12206 12207 12208 12209 12210 12211 12212 12213 12214 12215 12216 12217 12218 12219 12220 12221 12222 12223 12224 12222 12223 12224 12225 12228 12228 12229 12230 12231 12232 12233 12234 12233 12234 12235	000000000000000000000000000000000000000	HOH HOH HOH HOH HOH HOH HOH HOH HOH HOH	114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 140 141 142 143 144 145 146 147 148	41. 491 58. 601 0. 047 1. 00 42. 91 W 64. 362 64. 567 16. 259 1. 00 24. 97 W 43. 928 76. 242 2. 332 1. 00 21. 69 W 80. 703 69. 349 43. 827 1. 00 28. 64 W 81. 671 48. 368 20. 456 1. 00 15. 16 W 59. 413 71. 127 54. 004 1. 00 22. 01 W 27. 474 69. 426 47. 288 1. 00 26. 74 W 69. 871 60. 279 33. 380 1. 00 13. 47 W 67. 879 38. 425 47. 297 1. 00 25. 68 W 41. 866 62. 152 36. 306 1. 00 27. 91 W 82. 055 50. 923 20. 718 1. 00 23. 09 W 38. 821 82. 651 33. 998 1. 00 14. 04 W 64. 420 42. 195 31. 710 1. 00 28. 88 W 60. 713 36. 262 43. 885 1. 00 22. 95 W 63. 095 38. 041 44. 744 1. 00 26. 42 W 36. 718 65. 633 50. 633 1. 00 38. 12 W 36. 718 65. 633 50. 633 1. 00 38. 12 W 36. 718 65. 633 50. 633 1. 00 36. 38 W 75. 617 59. 792 32. 116 1. 00 26. 23 W 41. 981 65. 129 15. 577 1. 00 23. 62 W 48. 067 75. 632 53. 563 1. 00 36. 38 W 75. 617 59. 792 32. 116 1. 00 35. 58 W 73. 522 67. 486 30. 484 1. 00 21. 07 W 65. 965 81. 671 30. 091 1. 00 41. 74 W 41. 663 53. 300 13. 574 1. 00 39. 95 W 42. 885 39. 029 29. 960 1. 00 29. 57 W 67. 606 56. 683 24. 253 1. 00 37. 19 W 138. 150 54. 591 37. 133 1. 00 19. 60 W 76. 640 48. 505 51. 547 1. 00 22. 87 W 105. 346 35. 319 45. 478 1. 00 6. 28 W 108. 946 33. 058 43. 850 1. 00 17. 18 W 101. 384 50. 291 32. 321 1. 00 12. 25 W 83. 691 56. 732 33. 886 1. 00 18. 52 W 96. 721 59. 108 34. 335 1. 00 14. 59 W 122. 411 66. 436 57. 099 1. 00 19. 53 W 107. 303 38. 674 48. 678 1. 00 12. 12	(Continued) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
ATOM	12234		HOH	147	107. 303 38. 674 48. 678 1. 00 12. 12 W	
ATOM ATOM ATOM ATOM	12237 12238 12239 12240	0 0 0	HOH HOH HOH HOH	150 151 152 153	113. 995 67. 497 30. 740 1. 00 26. 00 W 115. 903 54. 147 45. 005 1. 00 10. 46 114. 104 55. 650 9. 401 1. 00 27. 03 W 86. 360 55. 414 40. 305 1. 00 14. 32 W	0 0 0 0
ATOM ATOM ATOM ATOM	12241 12242 12243 12244	0 0 0	HOH HOH HOH HOH	154 155 156 157	97. 554 40. 670 45. 200 1. 00 18. 35 W 119. 087 37. 761 27. 531 1. 00 31. 02 W 87. 809 62. 914 36. 962 1. 00 26. 29 W 83. 356 65. 229 44. 012 1. 00 37. 02 W	0 0 0 0
MOTA ATOM ATOM ATOM	12245 12246 12247 12248	0 0 0 0	HOH HOH HOH	158 159 160 161	98. 650 46. 435 54. 377 1. 00 26. 11 W 99. 982 40. 104 43. 504 1. 00 11. 71 W 122. 550 42. 243 44. 636 1. 00 14. 84 W 101. 404 56. 669 35. 498 1. 00 35. 54 W	0 0 0 0
ATOM	12249	0	НОН	162	88. 481 51. 896 31. 163 1. 00 12. 64 W	0

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										(Continued)
					FIG	. 4 -	2 5 1			(00111111111111111111111111111111111111
ATOM	12250	0	НОН	163	95. 169	58. 602	25.005	1. 00 10. 78	W	0
ATOM	12251	0	HOH	164		34.630	45.444	1.00 26.24	W	0
ATOM	12252	0	HOH	165		53.003	55.571	1.00 20.62	W	0
ATOM	12253	0	HOH	166		59. 299	19.482	1.00 36.24	W	0
ATOM	12254	0	HOH	167		50.670	46. 942	1.00 20.56	W	0
ATOM	12255	0	НОН	168		48. 091	37. 270	1.00 21.34	Ŋ	0
ATOM	12256	0	НОН	169		72. 537	31.569	1.00 23.37	Ä	0
ATOM	12257	0	HOH	170		58. 106	48.086	1.00 18.43	Ā	0
ATOM	12258	0	НОН	171		33. 853	32. 584	1.00 22.93	W	0
ATOM	12259	0	HOH	172		32. 367	28. 628	1.00 23.01	W	0
ATOM	12260	0	HOH	173		56. 523	56.950	1.00 35.07	W	0
ATOM	12261	0	HOH	174		59.050	11.178	1.00 23.37	W	0
ATOM ATOM	12262 12263	0	НОН	175		47. 759	51.786	1.00 19.27	W	0
ATOM	12264	0	НОН НОН	176 177		58. 234 64: 613	55. 683 44. 832	1.00 19.54 1.00 25.55	₩ ₩	0
ATOM	12265	0	HOH	178		67. 790	27. 707	1.00 29.36	W	0 0
ATOM	12266	0	НОН	179		40. 760	23. 388	1.00 28.01	Ÿ	0
ATOM	12267	ő	НОН	180		38. 188	50. 278	1.00 26.01	W	0
ATOM	12268	ŏ	НОН	181		40. 289	29. 465	1.00 7.47	Ÿ	Ŏ
ATOM	12269	ŏ	НОН	182		42. 102	29. 409	1.00 28.14	W	ŏ
ATOM	12270	Ŏ	НОН	183		33. 279	45. 877	1.00 22.55	Ÿ	ŏ
ATOM	12271	Ŏ	НОН	184		45. 858	44.078	1.00 28.83	W	Ŏ
ATOM	12272	0	HOH	185		38. 023	29.778	1.00 31.97	W	0
ATOM	12273	0	HOH -	186	122. 283	37. 257	34.566	1.00 18.77	W	0
ATOM	12274	0	HOH	187		38. 623	40.032	1.00 18.28	W	0
ATOM	12275	0	HOH	188		56.954	36. 341	1.00 20.05	W	0
ATOM	12276	0	HOH	189		78. 219	33.025	1.00 38.49	W	0
ATOM	12277	0	НОН	190		46.667	45.989	1.00 34.45	₩	0
ATOM	12278	0	НОН	191		39. 354	35. 865	1.00 10.27	W	0
ATOM	12279	0	НОН	192		51.843	57. 881	1.00 13.62	W	0
ATOM	12280	0	HOH	193		35. 631	32. 830	1.00 19.19	<u> </u>	0
ATOM	12281	0	НОН	194		45. 123	38. 393	1.00 26.68	Ä	0
ATOM	12282	0	HOH	195		60.696	63. 937	1.00 24.15	W	0
ATOM	12283 12284	0	HOH	196		59.856	31.652	1.00 12.71	W	0
ATOM ATOM	12285	0	НОН НОН	197		56. 246	54. 587	1.00 10.61	W	0
ATOM	12286	Ö	НОН	198 199		41. 219 75. 649	37. 675 27. 926	1.00 19.28	W	0
ATOM	12287	ő	НОН	200		44. 373	34. 046	1.00 9.03 1.00 8.20	W	0
ATOM	12288	Ö	НОН	201		44. 873	53. 124	1.00 8.20	W	0 0
ATOM	12289	ŏ	НОН	202		58. 341	13. 499	1.00 13.31	Ÿ	0
ATOM	12290	ő	НОН	203		39. 089	47. 689	1.00 22.63	₩	0
ATOM	12291	ŏ	HOH	204		54. 200	16.885	1.00 12.00	Ψ̈́	0
ATOM	12292	ŏ	НОН	205		34. 351	33. 261	1.00 15.83	Ÿ	0
ATOM	12293	ŏ	НОН	206		38. 178	46. 273	1.00 17.78	Ÿ	Ő
ATOM	12294	Ŏ	НОН	207		63. 592	15. 944	1.00 23.96	Ÿ	ŏ
ATOM	12295	Ö	HOH	208		52. 027	44. 587	1.00 12.16	Ÿ	ŏ
ATOM	12296	0	HOH	209		49. 450	36.803	1.00 19.70	Ÿ	Ö
ATOM	12297	0	HOH	210	78. 079	55. 141	59.990	1.00 33.63	Ÿ	Ö
ATOM	12298	0	HOH	211	95. 004	41.032	14. 678	1.00 29.66	W	0

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										(Continued)
					FIC	G. 4-	252			(Continued)
ATOM	10000	^	mon	010	110 '170	00 010	40 047	1 00 91 00	W	0
ATOM	12299	0	HOH	212	113.170	36.816	43. 347	1.00 21.90	W	0
ATOM	12300	0	HOH	213	77.770	71. 277 66. 746	45. 572 61. 783	1.00 31.73 1.00 37.87	₩	0 0
ATOM	12301	0	НОН НОН	214	128.636 128.566	42. 261	18. 644	1.00 31.61	Ϋ́	0
ATOM	12302	0		215 216	135.349	43. 830	34. 280	1.00 20.03	Ÿ	0
ATOM ATOM	12303 12304	0	HOH HOH	217	85. 640	67. 686	27. 706	1.00 24.03	W	0
ATOM	12304	0	НОН	218	93.669	46. 427	45. 506	1.00 24.39	Ÿ	0
ATOM	12306	0	НОН	219	117.990	67. 819	59.317	1.00 20.28	Ϋ́	Ö
ATOM	12307	Ö	НОН	220	79. 954	55. 009	62. 309	1.00 20.23	W	Ö
ATOM	12308	Ö	НОН	221	117. 228	62. 083	29. 483	1.00 29.50	Ÿ	ő
ATOM	12309	Ŏ	НОН	222	105.505	51. 938	31.912	1.00 35.19	Ÿ	Ö
ATOM	12310	ŏ	НОН	223	106.835	57. 215	14. 677	1.00 21.77	Ÿ	ŏ
ATOM	12311	Ö	НОН	224	107. 489	60. 380	64. 395	1.00 24.53	Ÿ	Ö
ATOM	12312	Ŏ	HOH	225	79. 753	74. 355	37. 799	1.00 35.35	W	Ö
ATOM	12313	Ŏ	НОН	226	116.807	64.679	29.466	1.00 24.83	W	0
ATOM	12314	0	НОН	227	87. 239	52.355	64.706	1.00 21.19	W	0
ATOM	12315	0	HOH	228	81.916	67. 988	41.878	1.00 14.54	W	0
ATOM	12316	0	HOH	229	106. 295	62. 226	36.826	1.00 26.06	W	0
ATOM	12317	0	HOH	230	78.057	49. 553	53.991	1.00 15.40	W	0
ATOM	12318	0	HOH	231	99. 797	47.673	22.572	1.00 18.00	W	0
ATOM	12319	0	HOH	232	80. 925	62.495	37. 326	1.00 9.28	W	0
ATOM	12320	0	HOH	233	93. 378	45.857	52. 934	1.00 12.13	W	0
ATOM	12321	0	HOH	234	132.069	46.877	33. 339	1.00 20.97	W	0
ATOM	12322	0	HOH	235	93.916	62.211	25. 521	1.00 13.10	W	0
ATOM	12323	0	HOH	236	93. 249	60. 882	37. 895	1.00 26.19	W	0
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WO 2004/011640 PCT/JP2003/009523

7/11

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Ile	Leu	Pro	Pro	His	Phe	Asp	Lys	Ser	Lys	Lys	Tyr	Pro	Leu	Leu	Leu
	530					535					540				
Asp	Val	Tyr	Ala	Gly	Pro	Cys	Ser	Gln	Lys	Ala	Asp	Thr	Val	Phe	Arg
545					550					555					560
Leu	Asn	Trp	Ala	Thr	Tyr	Leu	Ala	Ser	Thr	Glu	Asn	Ile	Ile	Val	Ala
				565					570					575	
Ser	Phe	Asp	Gly	Arg	Gly	Ser	Gly	Tyr	Gln	Gly	Asp	Lys	Ile	Met	His
			580					585					590		
Ala	Ile	Asn	Arg	Arg	Leu	Gly	Thr	Phe	Glu	Val	Glu	Asp	Gln	Ile	Glu
		595					600					605			
Ala	Ala	Arg	Gln	Phe	Ser	Lys	Met	Gly	Phe	Val	Asp	Asn	Lys	Arg	Ile
	610					615					620				
Ala	Ile	Trp	Gly	Trp	Ser	Tyr	Gly	Gly	Tyr	Val	Thr	Ser	Met	Val	Leu
625					630					635	•				640
Gly	Ser	Gly	Ser	Gly	Val	Phe	Lys	Cys	Gly	He	Ala	Val	Ala	Pro	Val
				645					650					655	
Ser	Arg	Trp	Glu	Tyr	Tyr	Asp	Ser	Val	Tyr	Thr	Glu	Arg	Tyr	Met	Gly
			660					665					670		
Leu	Pro	Thr	Pro	Glu	Asp	Asn	Leu	Asp	His	Tyr	Arg	Asn	Ser	Thr	Val
		675					680					685			
Met	Ser	Arg	Ala	Glu	Asn	Phe	Lys	Gln	Val	Glu	Tyr	Leu	Leu	Ile	His
	690					695					700				
Gly	Thr	Ala	Asp	Asp	Asn	Val	His	Phe	Gln	Gln	Ser	Ala	Gln	lle	Ser
705					710					715					720
Lys	Ala	Leu	Val	Asp	Val	Gly	Val	Asp	Phe	Gln	Ala	Me t	Trp	Tyr	Thr

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Asp Glu Asp His Gly Ile Ala Ser Ser Thr Ala His Gln His Ile Tyr 740 745 750

Thr His Met Ser His Phe Ile Lys Gln Cys Phe Ser Leu Pro

755 760 765

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A. CLASSIF IPC 7	FICATION OF SUBJECT MATTER C12N9/48 C07K14/705 G01N23/2	co G01N33/573	
According to	International Patent Classification (IPC) or to both national classifica-	ation and IPC	
B. FIELDS	SEARCHED		
Minimum do IPC 7	cumentation searched (classification system followed by classification $C12N - C07K - G01N$	on symbols)	
 	ion searched other than minimum documentation to the extent that s		
1	ata base consulted during the International search (name of data bas ternal, WPI Data, PAJ, BIOSIS, EMBAS)
C. DOCUME	ENTS CONSIDERED TO BE RELEVANT		
Category °	Citation of document, with indication, where appropriate, of the rel	evant passages	Relevant to claim No.
Х	KABASHIMA T ET AL: "DIPEPTIDYL F IV FROM XANTHAMONAS MALTOPHILIA: SEQUENCING AND EXPRESSION OF THE GENE AND CHARACTERIZATION OF THE ENZYME"	ENZYME	1,2,6
	JOURNAL OF BIOCHEMISTRY, JAPANESE BIOCHEMICAL SOCIETY, TOKYO, JP, vol. 120, no. 6, December 1996 (1 pages 1111-1117, XP000973151 ISSN: 0021-924X figure 4		
Υ	the whole document 	- /	3-5, 14-20
X Funt	ner documents are listed in the continuation of box C.	Patent family members are listed	in annex.
'A' docume consid 'E' earlier of filing d 'L' docume which citation 'O' docume other of the reference of the	tegories of cited documents: and defining the general state of the art which is not lered to be of particular relevance document but published on or after the international late and which may throw doubts on priority claim(s) or is cited to establish the publication date of another no rother special reason (as specified) and referring to an oral disclosure, use, exhibition or means and published prior to the international filing date but and the priority date claimed.	*T* later document published after the Inte or priority date and not in conflict with cited to understand the principle or the invention *X* document of particular relevance; the cannot be considered novel or cannot involve an inventive step when the document of particular relevance; the cannot be considered to involve an inventive step when the document is combined with one or moments, such combination being obvior in the art.	the application but every underlying the claimed invention to be considered to current is taken atone claimed invention ventive step when the one other such docu-us to a person skilled
	actual completion of the international search 9 November 2003	Date of mailing of the international second	arch report
Name and n	mailing address of the ISA European Patent Office, P.B. 5818 Patentlaan 2	Authorized officer	
	NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	Bucka, A	•

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Category *	DOCUMENTS CONSIDERED TO BE RELEVANT Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
γ	ARROTT CATHERINE A ET AL: "Binding to	3-5,
	human dipeptidyl peptidase IV by adenosine deaminase and antibodies that inhibit ligand binding involves overlapping, discontinuous sites on a predicted beta propeller domain" EUROPEAN JOURNAL OF BIOCHEMISTRY, vol. 266, no. 3, December 1999 (1999-12), pages 798-810, XP002261851 ISSN: 0014-2956 the whole document	14-20
1	LAMBEIR A-M ET AL: "A prediction of DPP IV/CD26 domain structure from a physico-chemical investigation of dipeptidyl peptidase IV (CD26) from human seminal plasma" BIOCHIMICA ET BIOPHYSICA ACTA. PROTEIN STRUCTURE AND MOLECULAR ENZYMOLOGY, ELSEVIER, AMSTERDAM, NL, vol. 1340, no. 2,	3-5, 14-20
	18 July 1997 (1997-07-18), pages 215-226, XP004281676 ISSN: 0167-4838 the whole document	
Υ .	MEDRANO F J ET AL: "Structure of proline iminopeptidase from Xanthomonas campestris pv. citri: A prototype for the prolyl oligopeptidase family" EMBO (EUROPEAN MOLECULAR BIOLOGY ORGANIZATION) JOURNAL, vol. 17, no. 1, 2 January 1998 (1998-01-02), pages 1-9, XP002261745 ISSN: 0261-4189 the whole document	3-5, 14-20
A	POLGAR L: "The prolyl oligopeptidase family" CMLS CELLULAR AND MOLECULAR LIFE SCIENCES, BIRKHAUSER VERLAG, BASEL, CH, vol. 59, no. 2, February 2002 (2002-02), pages 349-362, XP002219152 ISSN: 1420-682X the whole document	1-6, 14-20
А	FULOP V ET AL: "Prolyl oligopeptidase: An unusual beta-propeller domain regulates proteolysis" CELL, CELL PRESS, CAMBRIDGE, NA, US, vol. 94, no. 2, 24 July 1998 (1998-07-24), pages 161-170, XP002221331 ISSN: 0092-8674 the whole document	1-6, 14-20

Internation—Application No PCT/JP 03/09523

C/C	ation) DOCUMENTS CONSIDERED TO BE RELEVANT	
Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Jalegoly -	Change of accounting that management appropriately a second secon	
A	AUGUSTYNS K ET AL: "THE UNIQUE PROPERTIES OF DIPEPTIDYL-PEPTIDASE IV (DPP IV/CD26) AND THE THERAPEUTIC POTENTIAL OF DPP IV INHIBITORS" CURRENT MEDICINAL CHEMISTRY, BENTHAM SCIENCE PUBLISHERS BV, BE, vol. 6, no. 4, 1999, pages 311-327, XP000870290 ISSN: 0929-8673 the whole document	1-6, 14-20
P,X	ENGEL MICHAEL ET AL: "The crystal structure of dipeptidyl peptidase IV (CD26) reveals its functional regulation and enzymatic mechanism." PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES, vol. 100, no. 9, 29 April 2003 (2003-04-29), pages 5063-5068, XP002261746 April 29, 2003 / ISSN: 0027-8424 (ISSN print) the whole document	1-6, 14-20
P,X	RASMUSSEN HANNE B ET AL: "Crystal structure of human dipeptidyl peptidase IV/CD26 in complex with a substrate analog." NATURE STRUCTURAL BIOLOGY, vol. 10, no. 1, January 2003 (2003-01), pages 19-25, XP001168693 ISSN: 1072-8368 (ISSN print) the whole document	1-6, 14-20
P,X	HIRAMATSU HAJIME ET AL: "The structure and function of human dipeptidyl peptidase IV, possessing a unique eight-bladed beta-propeller fold." BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS, vol. 302, no. 4, 21 March 2003 (2003-03-21), pages 849-854, XP002261748 ISSN: 0006-291X the whole document	1-6, 14-20

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		PCT/JP 03/09523	
C.(Continu	ation) DOCUMENTS CONSIDERED TO BE RELEVANT		
Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim	n No.
P,X	OEFNER CHRISTIAN ET AL: "High-resolution structure of human apo dipeptidyl peptidase IV/CD26 and its complex with 1-'('2-'(5-iodopyridin-2-yl)amino!-ethyl!a mino)- acetyl!-2-cyano-(S)-pyrrolidine." ACTA CRYSTALLOGRAPHICA. SECTION D, BIOLOGICAL CRYSTALLOGRAPHY. DENMARK JUL 2003, vol. 59, no. Pt 7, July 2003 (2003-07), pages 1206-1212, XP008024791 ISSN: 0907-4449 the whole document	1-6, 14-20	
			·
1			

International application No. PCT/JP 03/09523

INTERNATIONAL SEARCH REPORT

Box I Observations where certain claims were found unsearchable (Continuation of Item 1 of first sheet)				
This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:				
1. X Claims Nos.: 7-13 22-24 because they relate to subject matter not required to be searched by this Authority, namely: see FURTHER INFORMATION sheet PCT/ISA/210				
2. Claims Nos.: because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically: see FURTHER INFORMATION sheet PCT/ISA/210				
3. Claims Nos.: because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).				
Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)				
This International Searching Authority found multiple inventions in this international application, as follows:				
As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.				
2. As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.				
3. As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:				
A. No required additional search fees were timely paid by the applicant. Consequently, this international Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:				
Remark on Protest The additional search fees were accompanied by the applicant's protest. No protest accompanied the payment of additional search fees.				

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.1

Claims Nos.: 7-13, 22-24

Concerning claims 7 to 13 and 22 to 24 applicant's attention is drawn to Rule 39.1(v) PCT.

The subject-matter of claims 7 to 13 and 22 to 24 refers only to the presentation of structural information and is not regarded as patentable invention within the meaning of Rule 39.1(v) PCT. This information is disclosed e. g. as the atomic coordinates listings (or Tables) of a model, their use in a non-technical method, or said information is stored on a diskette/computer.

Thus, the above mentioned claims will not be searched in accordance with Article 17(2)(a)(i) PCT.

Continuation of Box I.2

Claims Nos.: 21

Present claim 21 relates to a product, i. e. an "effector", defined by reference to a desirable characteristic or property, namely as being an effector of dipeptidyl peptidase IV.

The claim covers all products having this characteristic or property, whereas the application provides no support within the meaning of Article 6 PCT and no disclosure within the meaning of Article 5 PCT of any such products. In the present case, the claim so lacks support, and the application so lacks disclosure, that a meaningful search of the claim is impossible.

Independent of the above reasoning, the claim also lacks clarity (Article 6 PCT). An attempt is made to define the product by reference to a result to be achieved. Again, this lack of clarity in the present case is such as to render a meaningful search over the whole of the claimed scope impossible.

Consequently, no search has been carried out under the provisions of Article 17(2)(a)(ii) PCT.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.